```
=> fil reg; d stat que l32; d stat que l40
FILE 'REGISTRY' ENTERED AT 17:28:25 ON 30 MAR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   29 MAR 2005  HIGHEST RN 847544-86-9
DICTIONARY FILE UPDATES:  29 MAR 2005  HIGHEST RN 847544-86-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

*************************************************************************
*                                                                       *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                                       *
*************************************************************************

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html


L7              STR
```
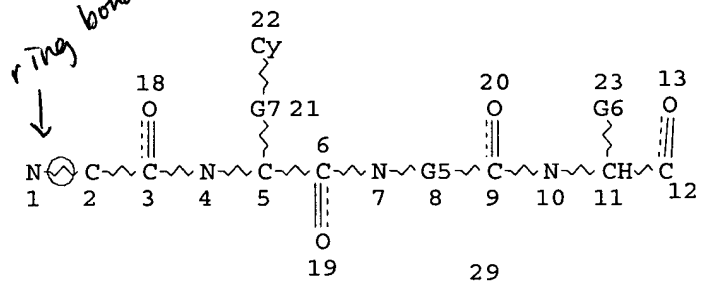
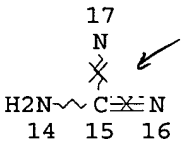
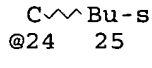
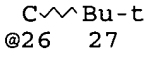

ring bonds & nodes

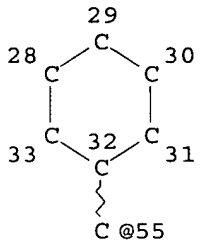


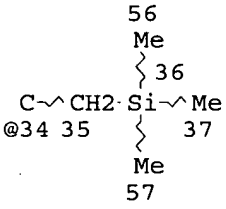
Ring or chain bonds & nodes

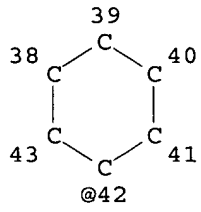


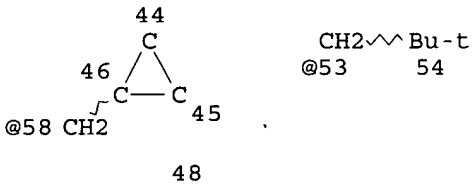




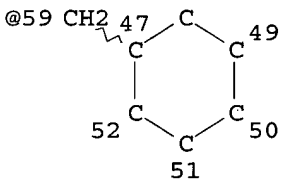








Page 1-A

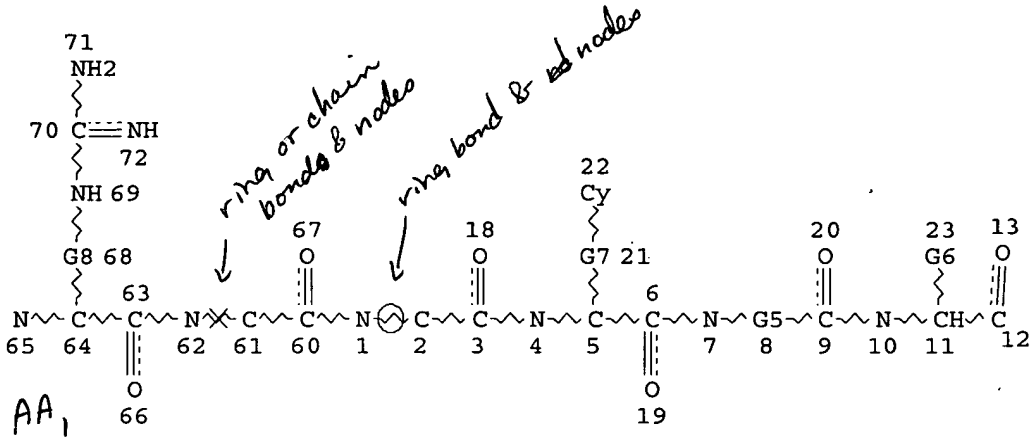


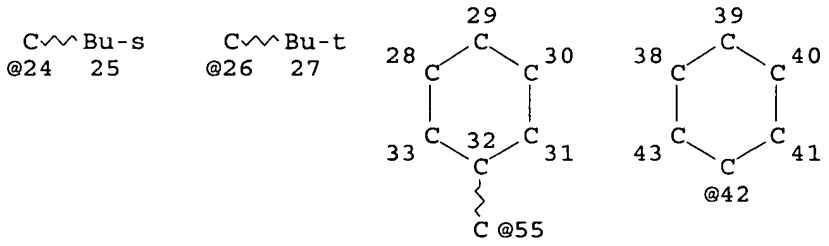
full file search done on this structure

Page 2-A
VAR G5=24/26/55/34/42
VAR G6=58/59/53/I-BU
REP G7=(0-5) CH2
NODE ATTRIBUTES:
NSPEC IS R AT 1
NSPEC IS R AT 2
NSPEC IS RC AT 15
NSPEC IS RC AT 16
NSPEC IS RC AT 17
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 22
DEFAULT ECLEVEL IS LIMITED

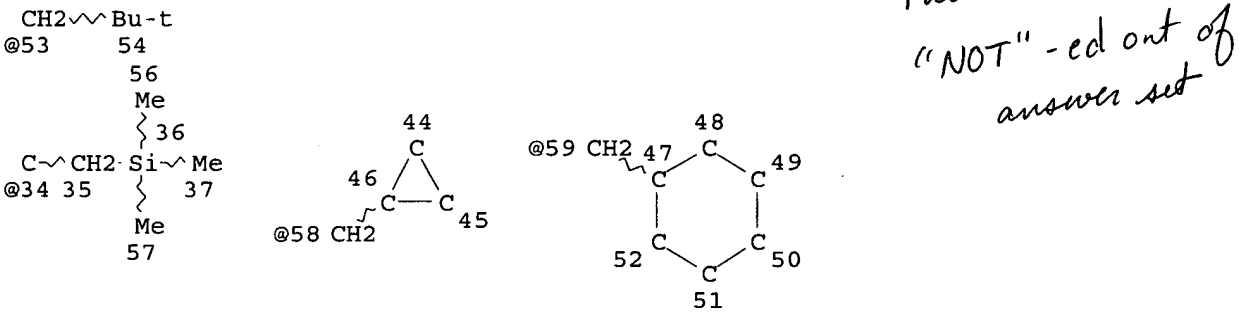
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 59

STEREO ATTRIBUTES: NONE
L11 STR





Page 1-A

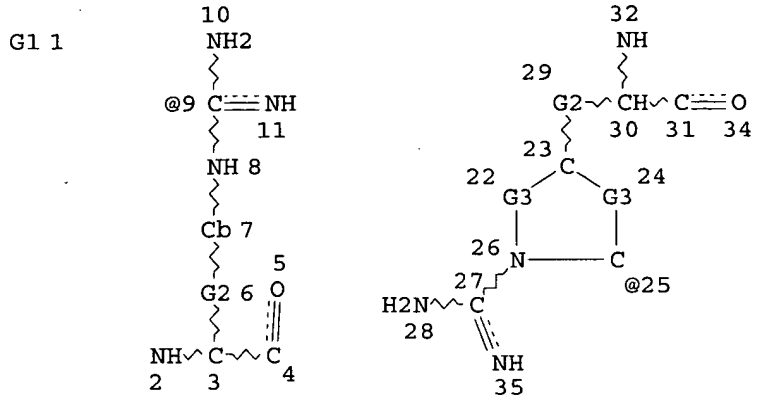


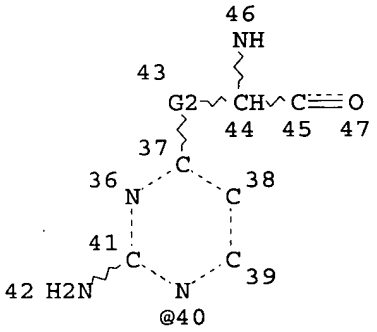
this structure "NOT"-ed out of answer set

Page 2-A
VAR G5=24/26/55/34/42
VAR G6=58/59/53/I-BU
REP G7=(0-5) CH2
REP G8=(3-3) CH2
NODE ATTRIBUTES:
NSPEC IS R AT 1
NSPEC IS R AT 2
NSPEC IS RC AT 61
NSPEC IS RC AT 62
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 22
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 68

STEREO ATTRIBUTES: NONE
L15 853 SEA FILE=REGISTRY SSS FUL L7
L16 STR





claim 2

VAR G1=9/25/40
REP G2=(0-6) CH2
REP G3=(1-7) CH2
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 36

STEREO ATTRIBUTES: NONE
L17 STR

1 A *

A = any atom, ring or chain, with abnormal mass

NODE ATTRIBUTES:
MASS IS * AT 1
NSPEC IS RC AT 1
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 1

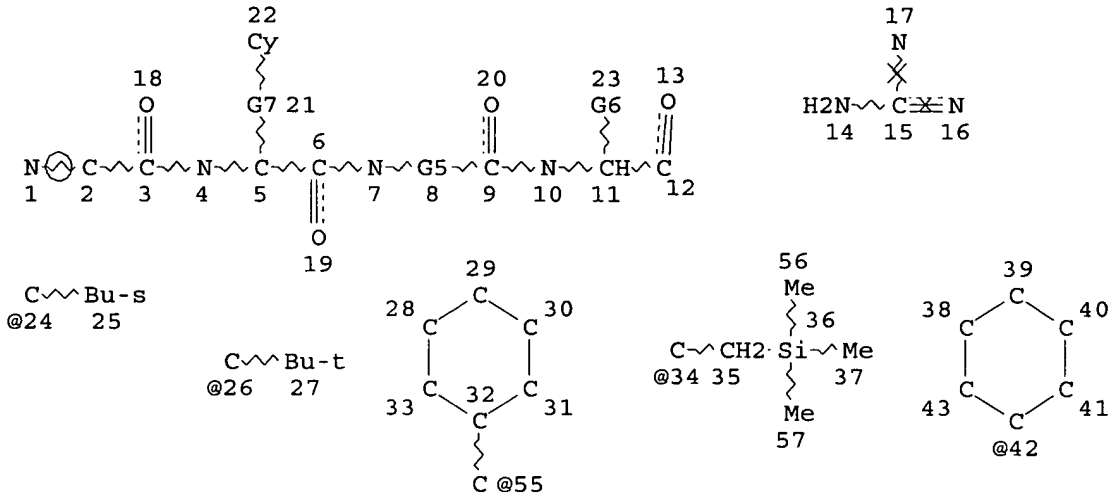
STEREO ATTRIBUTES: NONE

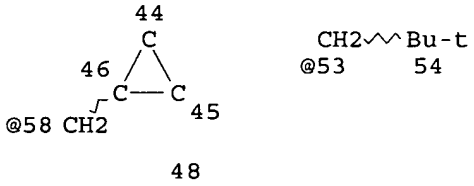
L32 30 SEA FILE=REGISTRY SUB=L15 SSS FUL (((L7 NOT L11) OR L16) AND L17)

all answers have at least 1 atom with abnormal mass

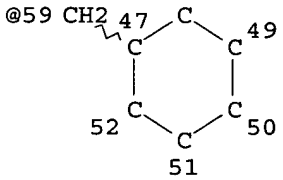
100.0% PROCESSED 853 ITERATIONS 30 ANSWERS
SEARCH TIME: 00.00.01

L7 STR





Page 1-A

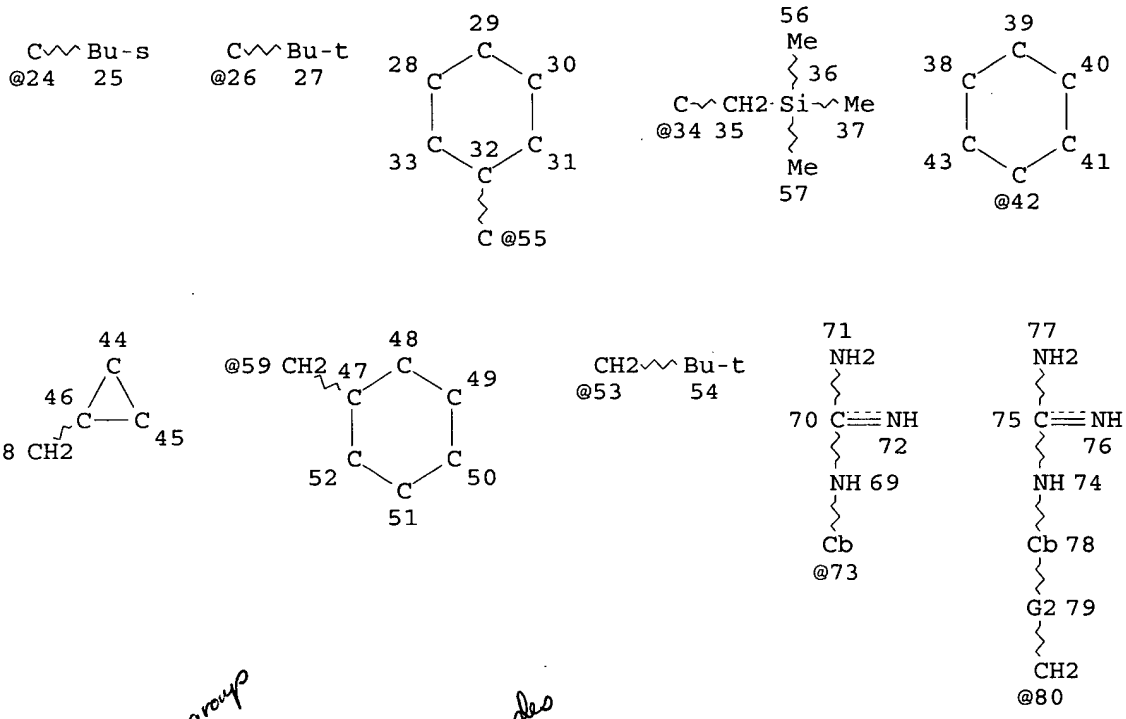


Page 2-A
VAR G5=24/26/55/34/42
VAR G6=58/59/53/I-BU
REP G7=(0-5) CH2
NODE ATTRIBUTES:
NSPEC IS R AT 1
NSPEC IS R AT 2
NSPEC IS RC AT 15
NSPEC IS RC AT 16
NSPEC IS RC AT 17
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 22

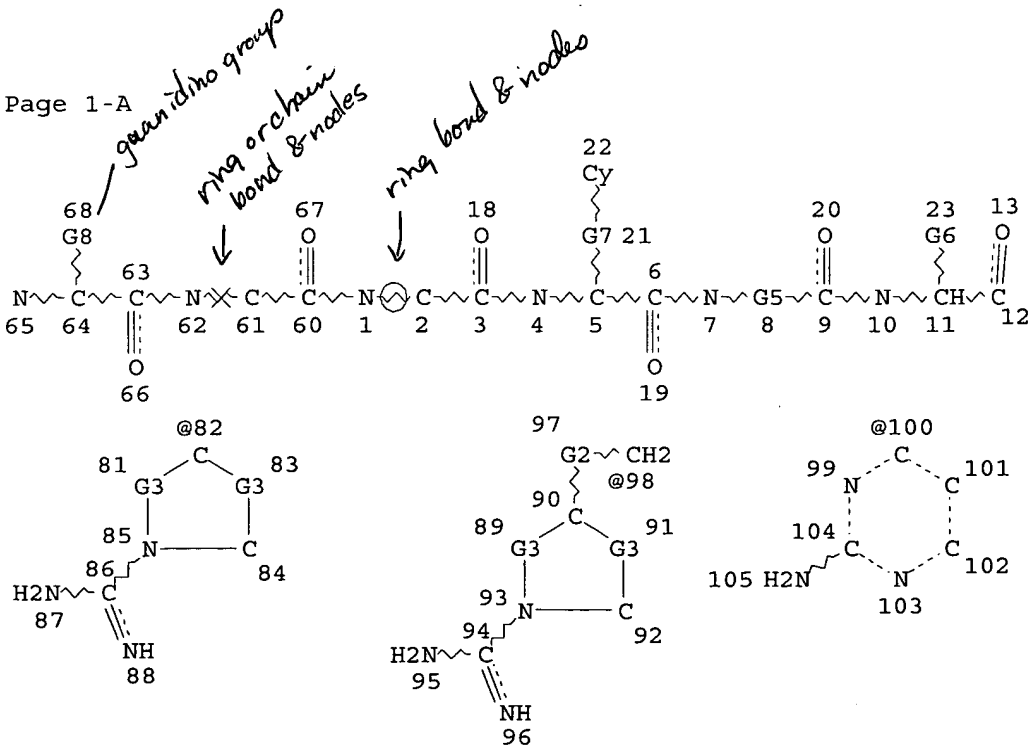
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 59

STEREO ATTRIBUTES: NONE
L15 853 SEA FILE=REGISTRY SSS FUL L7
L37 STR

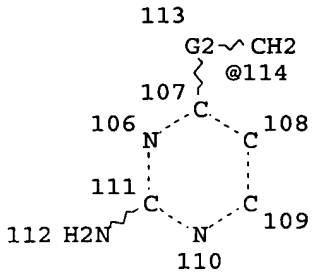


Page 1-A



2nd search done, forcing arginine mimics (guanidino group-containing structure) to be at position AA,

Page 2-A



Page 3-A
REP G2=(0-5) CH2
REP G3=(1-7) CH2
VAR G5=24/26/55/34/42
VAR G6=58/59/53/I-BU
REP G7=(0-5) CH2
VAR G8=73/80/82/98/100/114
NODE ATTRIBUTES:
NSPEC IS R AT 1
NSPEC IS R AT 2
NSPEC IS RC AT 61
NSPEC IS RC AT 62
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 22
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 110

STEREO ATTRIBUTES: NONE
L40 74 SEA FILE=REGISTRY SUB=L15 SSS FUL L37

100.0% PROCESSED 840 ITERATIONS 74 ANSWERS answers have guanidino group at position AA,
SEARCH TIME: 00.00.01

=> s l32 or l40
L43 84 L32 OR L40

=> fil capl toxcenter prousddr
FILE 'CAPLUS' ENTERED AT 17:28:52 ON 30 MAR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE 'TOXCENTER' ENTERED AT 17:28:52 ON 30 MAR 2005

FILE 'PROUSDDR' ENTERED AT 17:28:52 ON 30 MAR 2005

=> s l43
L44 16 L43

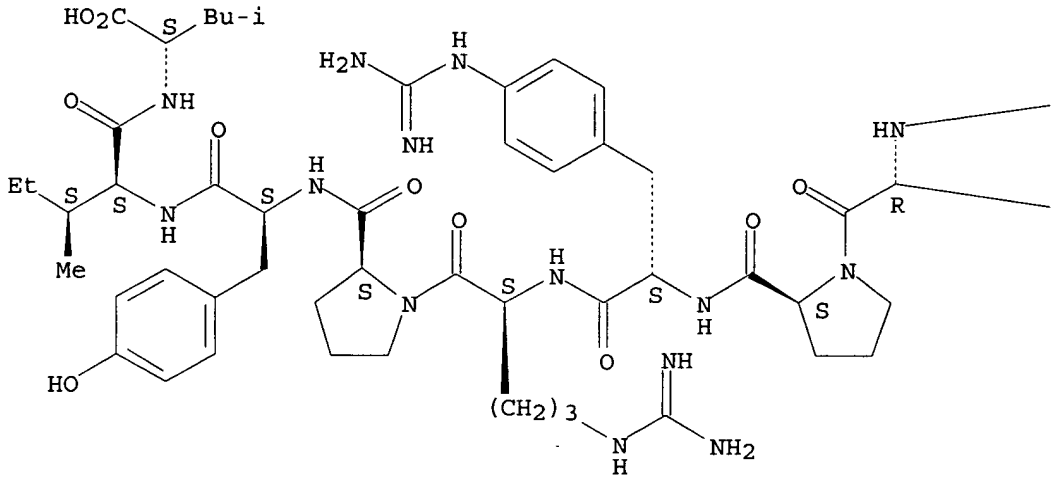
```
=> dup rem l44
DUPLICATE IS NOT AVAILABLE IN 'PROUSDDR'.
ANSWERS FROM THESE FILES WILL BE CONSIDERED UNIQUE
PROCESSING COMPLETED FOR L44
L45          11 DUP REM L44 (5 DUPLICATES REMOVED)
                ANSWERS '1-10' FROM FILE CAPLUS
                ANSWER '11' FROM FILE PROUSDDR

=> d ibib ed abs hitstr 1-10; d iall 11; fil hom

L45  ANSWER 1 OF 11  CAPLUS  COPYRIGHT 2005 ACS on STN DUPLICATE 1
ACCESSION NUMBER:         2003:469885  CAPLUS
DOCUMENT NUMBER:          139:185489
TITLE:                    Novel Bioactive and Stable Neurotensin Peptide Analogs
                          Capable of Delivering Radiopharmaceuticals and
                          Molecular Beacons to Tumors
AUTHOR(S):                Achilefu, Samuel; Srinivasan, Ananthacari; Schmidt,
                          Michelle A.; Jimenez, Hermo N.; Bugaj, Joseph E.;
                          Erion, Jack L.
CORPORATE SOURCE:         Mallinckrodt Institute of Radiology, Washington
                          University School of Medicine, St. Louis, MO, 63110,
                          USA
SOURCE:                   Journal of Medicinal Chemistry (2003), 46(15),
                          3403-3411
                          CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER:                American Chemical Society
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
ED   Entered STN:  20 Jun 2003
AB   The prevalence of neurotensin receptor (NTR) in several human tumors makes
     it an attractive target for the delivery of cytotoxic drugs and imaging
     agents.  Native neurotensin (NT) is a tridecapeptide that binds to NTR and
     induces tumor growth. Unfortunately, NT has a short plasma half-life,
     which hinders its use for in vivo biomedical applications.  Numerous
     reports suggest that Arg(8)-Arg(9) and Tyr(11)-Ile(12) amide bonds are
     particularly susceptible to degradation by proteolytic enzymes.  Predicated on
     this observation, we substituted Arg(8), Arg(9), and Ile(12) amino acids
     with the corresponding com. available mimics.  These surrogate amino acids
     are amenable to standard Fmoc peptide synthesis strategy, and the resulting
     compds. are stable in biol. media for >4 h and bind to NTR with high
     affinity.  Furthermore, conjugating DTPA to the new peptides and
     subsequent labeling with 111In-DTPA for nuclear imaging or fluorescein for
     optical imaging did not diminish the NTR binding affinities of the
     peptides.  In vivo biodistribution of a representative 111In-DTPA-NT
     peptide analog in SCID mice bearing NTR-pos. human adenocarcinoma (HT29)
     xenograft shows that the compound was primarily retained in tumor tissue
     (2.2% ID/g) and the kidneys (4.8% ID/g) at 4 h postinjection.  Coinjection
     of cold NT and the radiolabeled NT peptide analog inhibited the tumor but
     not the kidney uptake, demonstrating that retention of the radiolabeled
     compound in tumor tissue was mediated by NTR specific uptake while it
     accumulates in the kidneys by a nonspecific mechanism.  These findings
     show that the new NT peptide analogs are robust and can deliver imaging
     agents to NTR-pos. tumors such as pancreatic cancer.
IT   578719-69-4P 578719-72-9P 578719-74-1P
     578719-80-9P 578719-82-1P 578719-84-3P
     578719-86-5P 578719-88-7P 578719-90-1P
     578719-92-3P 578719-94-5P 578719-96-7P
     578719-98-9P 578720-00-0P 578720-02-2P
     578720-06-6P 578720-08-8P 578720-10-2P
     578720-12-4P 579448-97-8P 579448-98-9P
```

579448-99-0P 579449-00-6P 579449-01-7P
579449-02-8P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(novel bioactive and stable neurotensin peptide analogs capable of delivering radiopharmaceuticals and mol. beacons to tumors)

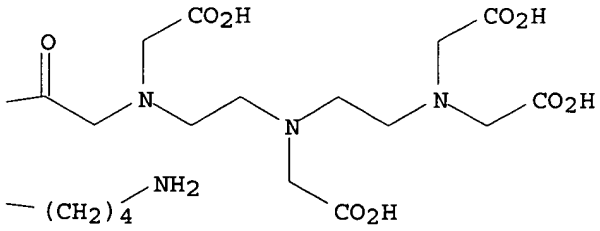
RN 578719-69-4 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-4-[(aminoiminomethyl)amino]-L-phenylalanyl-L-arginyl-L-prolyl-L-tyrosyl-L-isoleucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



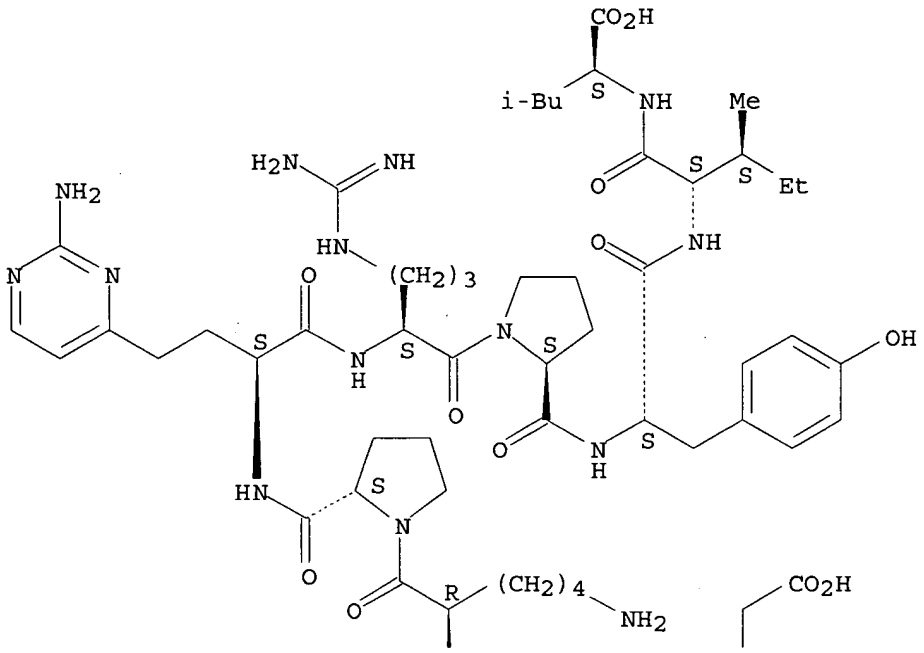
PAGE 1-B



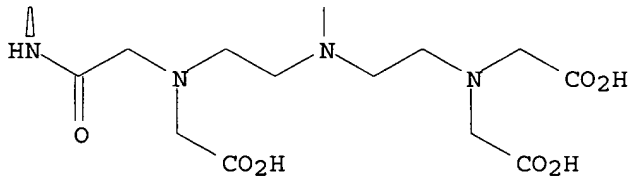
RN 578719-72-9 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-(αS)-α,2-diamino-4-pyrimidinebutanoyl-L-arginyl-L-prolyl-L-tyrosyl-L-isoleucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



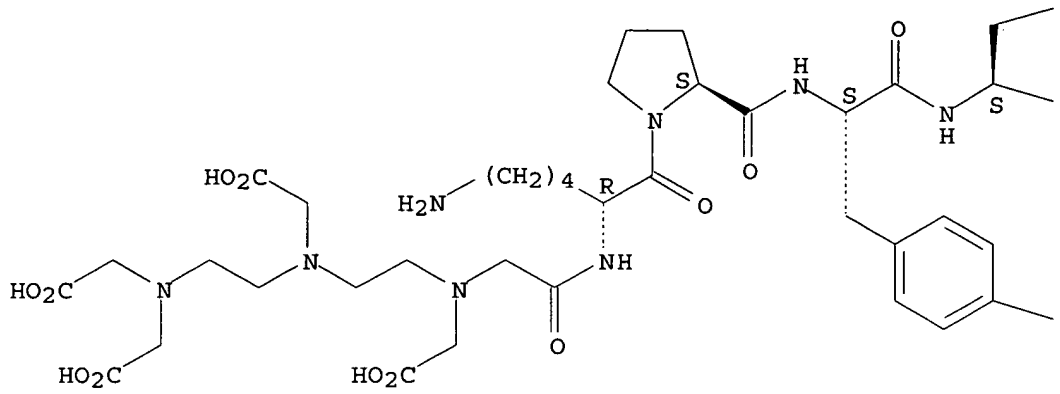
PAGE 2-A



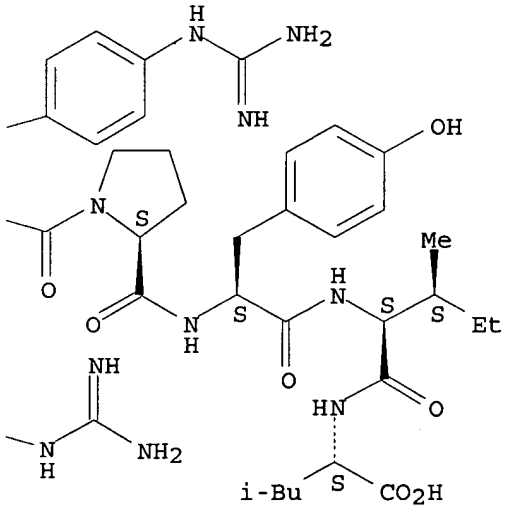
RN 578719-74-1 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-4-[(aminoiminomethyl)amino]-L-phenylalanyl-4-[(aminoiminomethyl)amino]-L-phenylalanyl-L-prolyl-L-tyrosyl-L-isoleucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



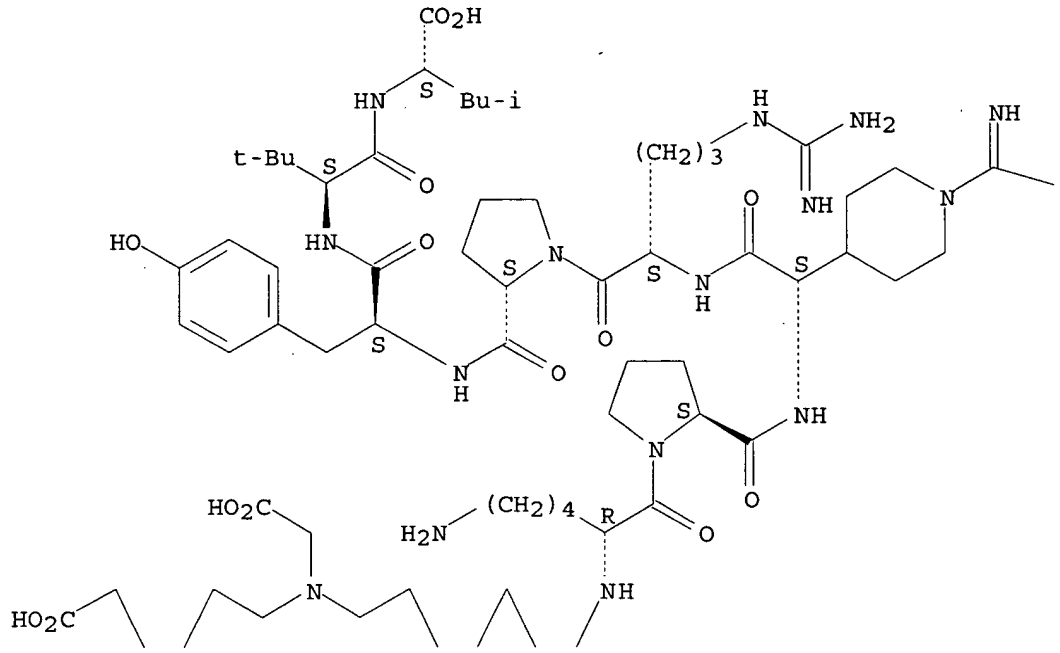
PAGE 1-B



RN 578719-80-9 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-(2S)-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methyl-L-valyl- (9CI) (CA INDEX NAME)

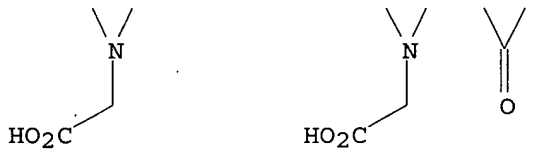
Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

PAGE 2-A

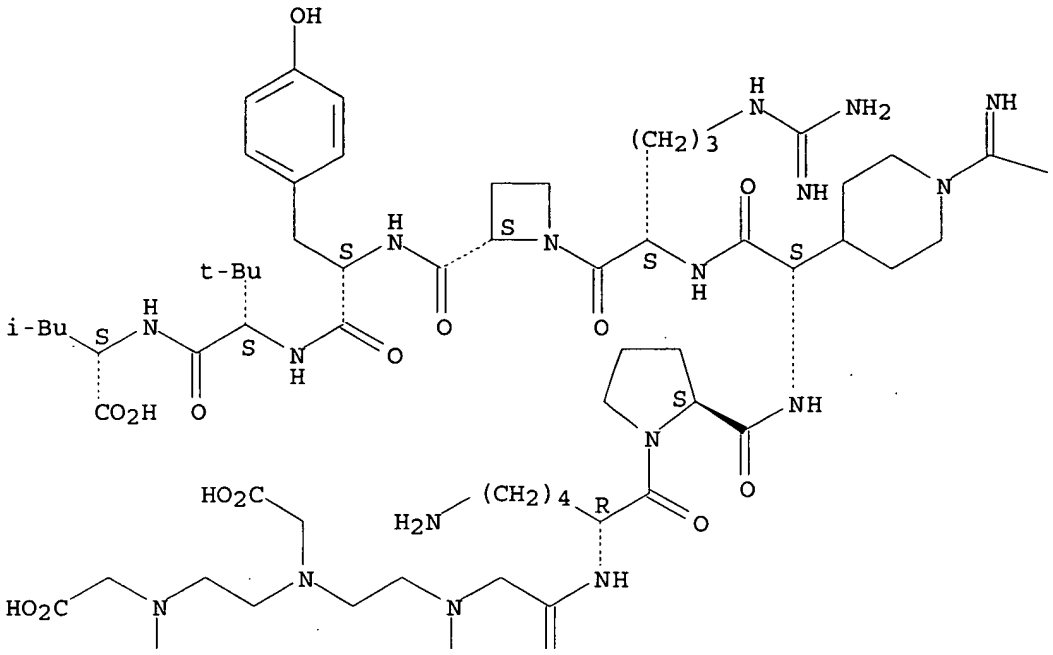


RN 578719-82-1 CAPLUS

CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-(2S)-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-(2S)-2-azetidinecarbonyl-L-tyrosyl-3-methyl-L-valyl- (9CI) (CA INDEX NAME)

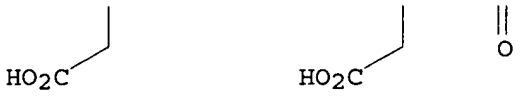
Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

PAGE 2-A

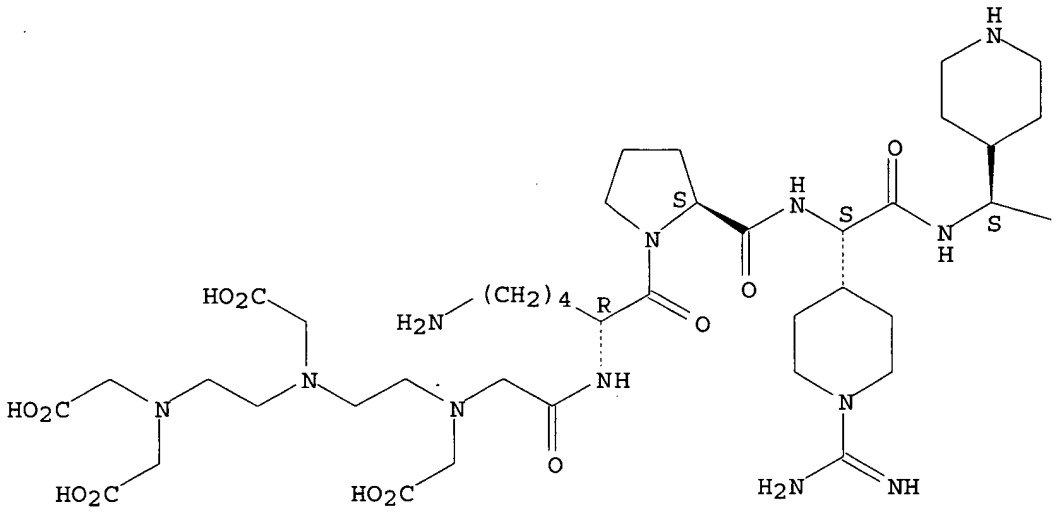


RN 578719-84-3 CAPLUS

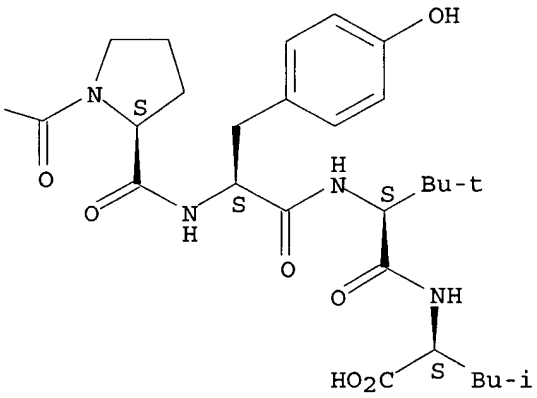
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-(2S)-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-(2S)-2-(4-piperidinyl)glycyl-L-prolyl-L-tyrosyl-3-methyl-L-valyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



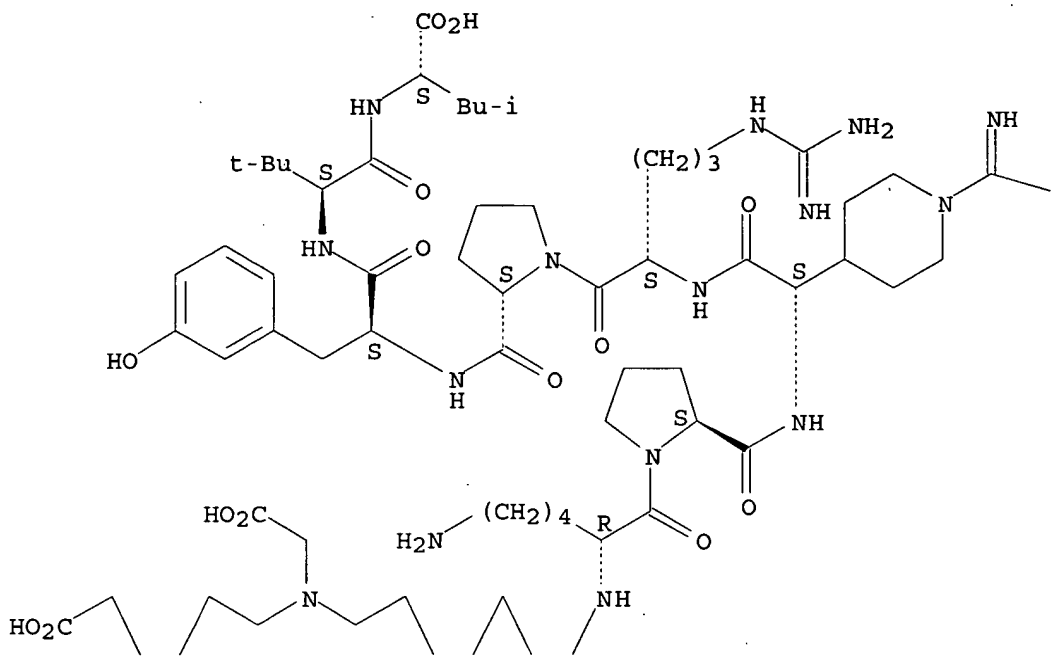
PAGE 1-B



RN 578719-86-5 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-(2S)-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-3-hydroxy-L-phenylalanyl-3-methyl-L-valyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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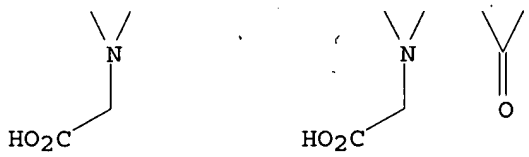
PAGE 2-A

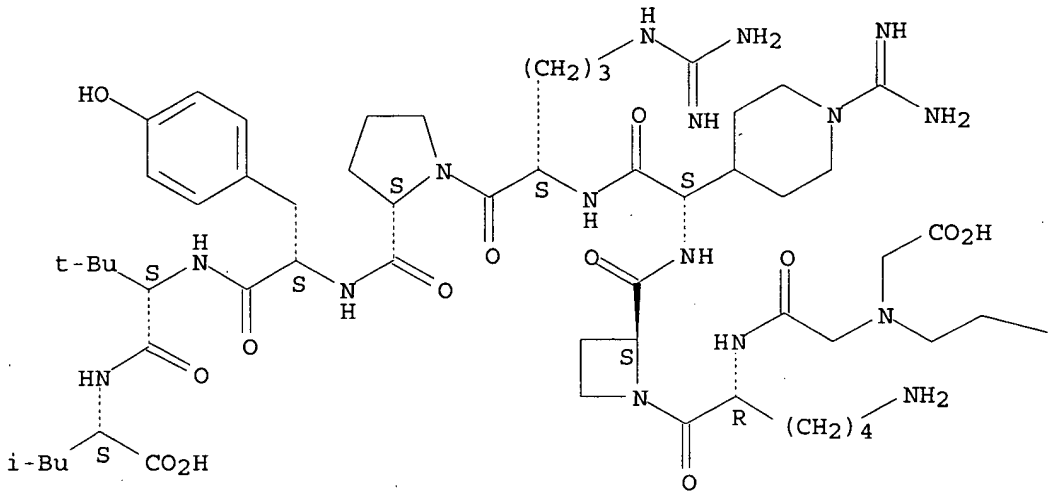


RN 578719-88-7 CAPLUS

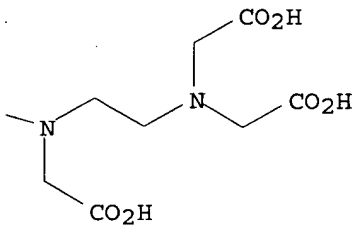
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-(2S)-2-azetidinecarbonyl-(2S)-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methyl-L-valyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



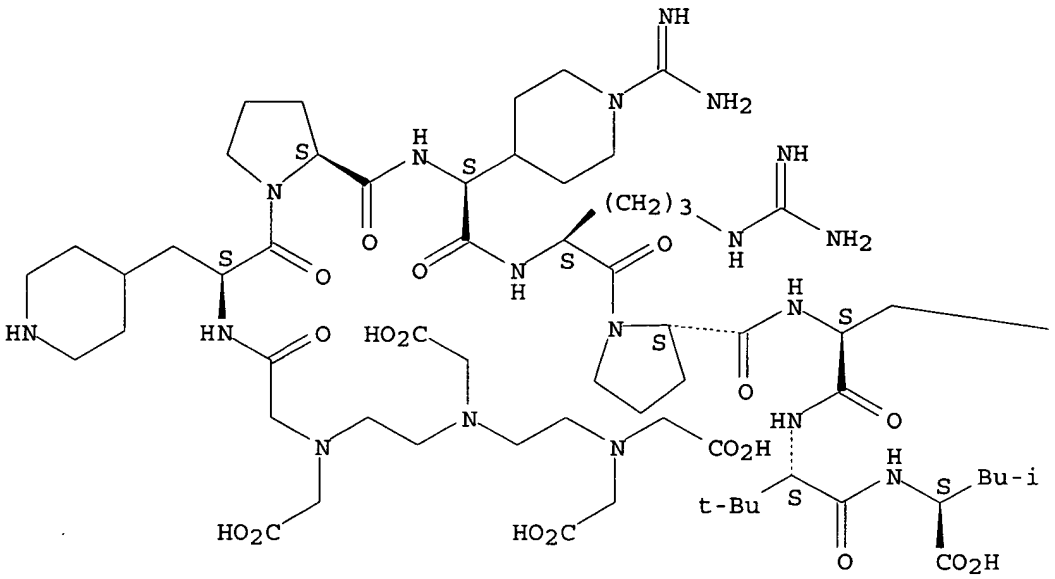
PAGE 1-B



RN 578719-90-1 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-3-(4-piperidinyl)-L-alanyl-L-prolyl-(2S)-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methyl-L-valyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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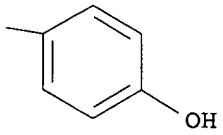
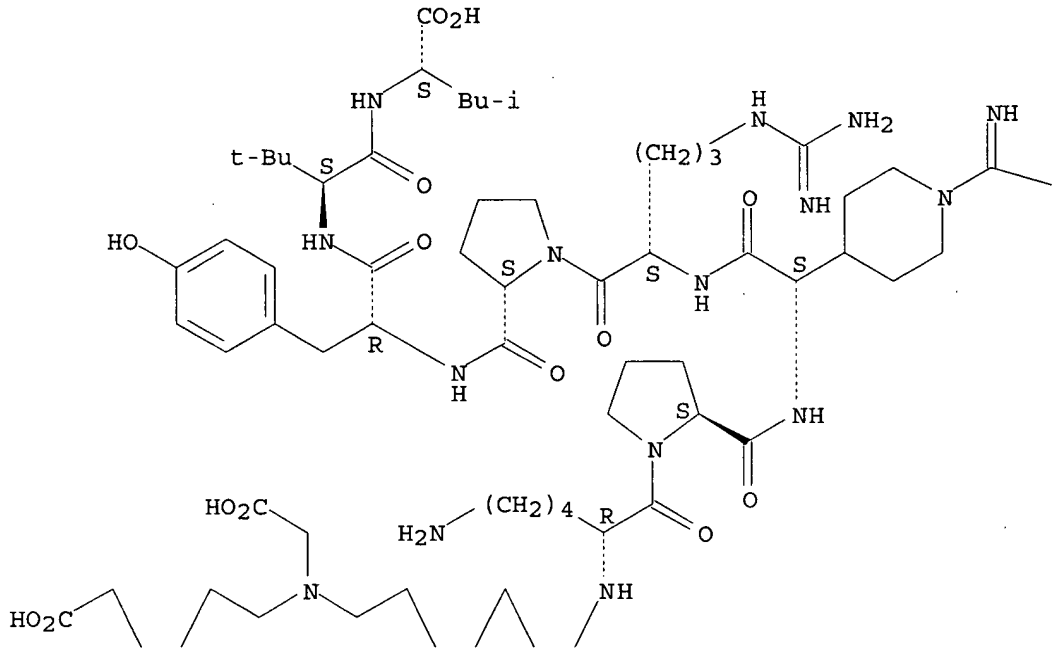


RN 578719-92-3 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-(2S)-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-D-tyrosyl-3-methyl-L-valyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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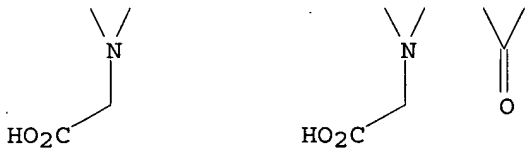
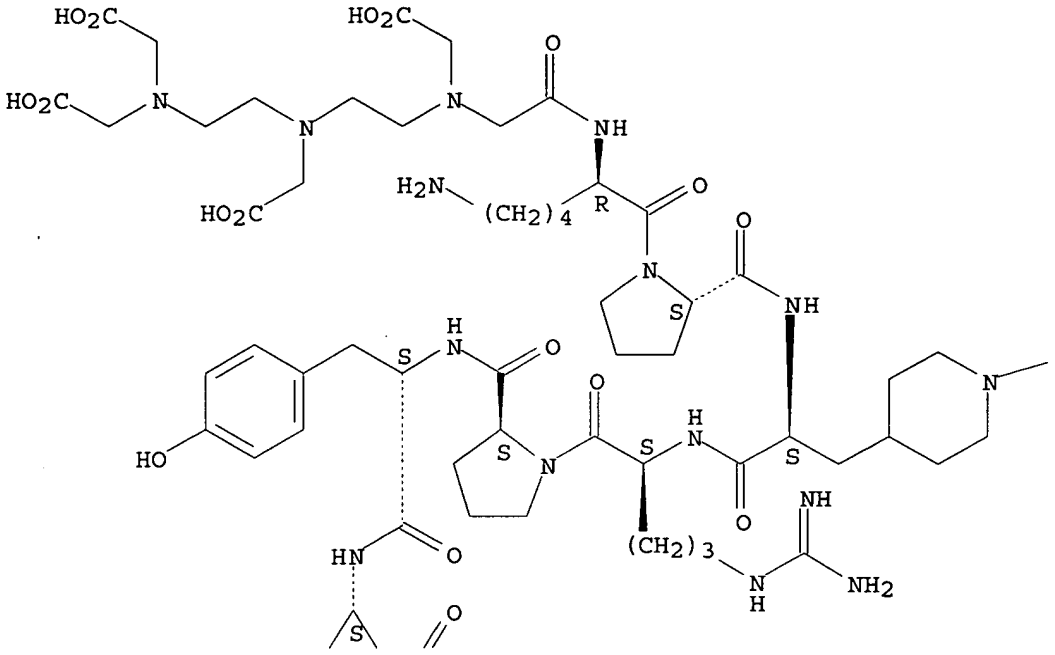
PAGE 2-A



RN 578719-94-5 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-(2S)-3-[1-(aminoiminomethyl)-4-piperidinyl]alanyl-L-arginyl-L-prolyl-L-tyrosyl-3-methyl-L-valyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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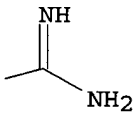

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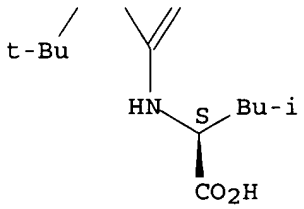
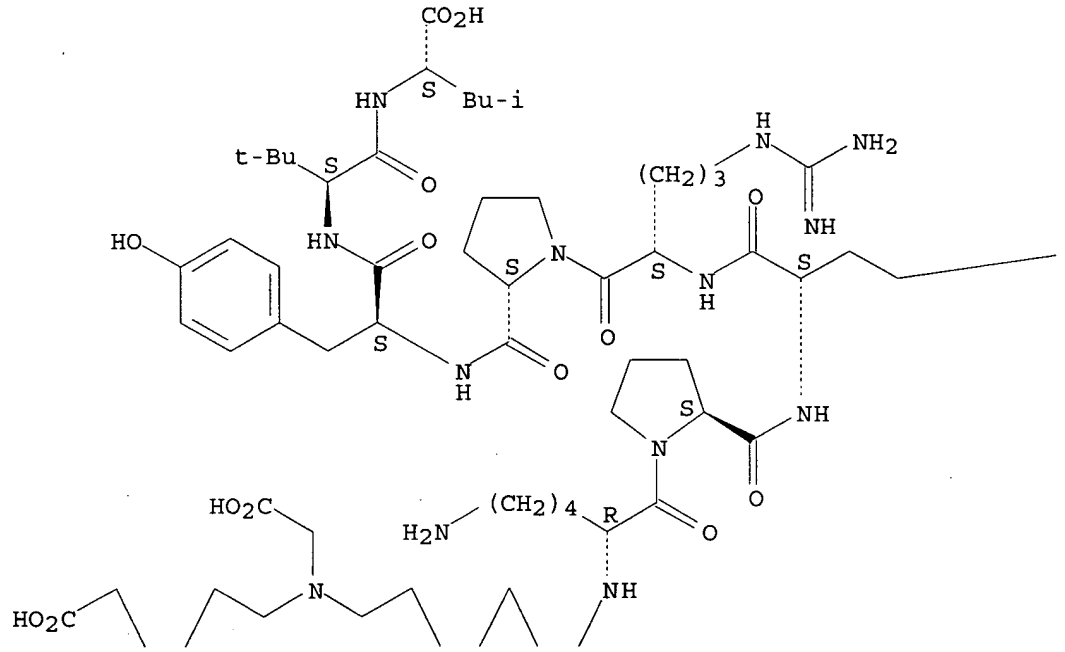


Searched by Barb O'Bryen, STIC 2-2518

RN 578719-96-7 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-(αS)-α-amino-1-(aminoiminomethyl)-4-piperidinebutanoyl-L-arginyl-L-prolyl-L-tyrosyl-3-methyl-L-valyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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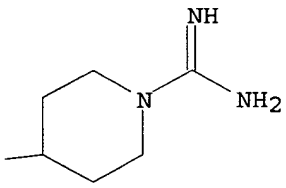

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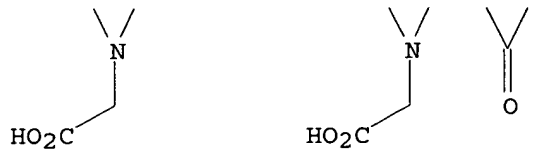
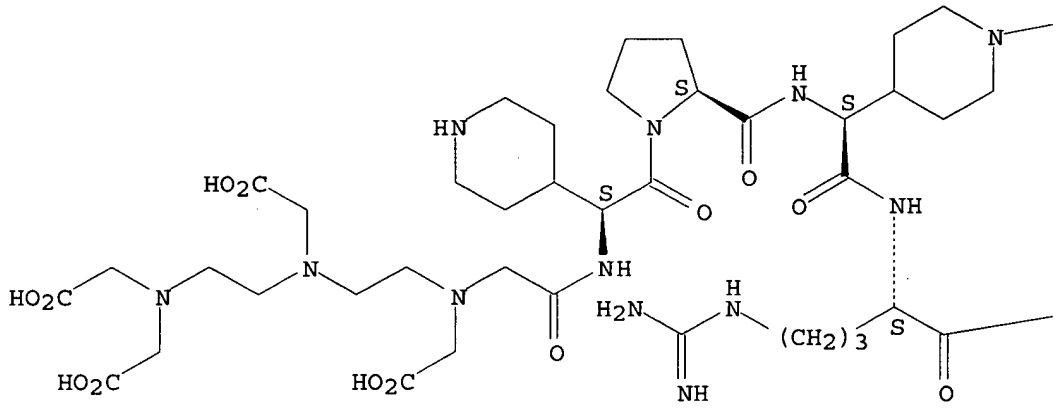


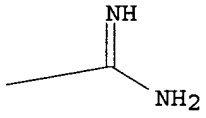
RN 578719-98-9 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-(2S)-2-(4-piperidinyl)glycyl-L-prolyl-(2S)-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methyl-L-valyl- (9CI) (CA INDEX NAME)

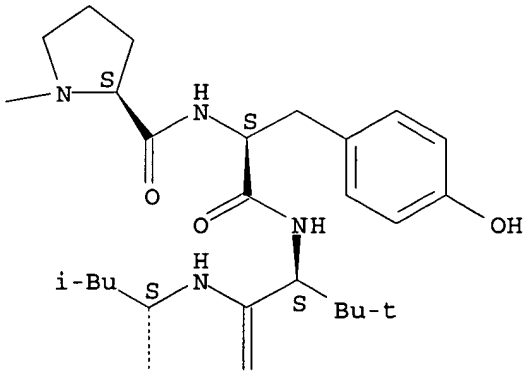
Absolute stereochemistry.

PAGE 1-A



PAGE 1-B





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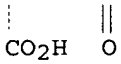

RN 578720-00-0 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-3-[trans-4-(aminomethyl)cyclohexyl]-L-alanyl-L-prolyl-(2S)-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methyl-L-valyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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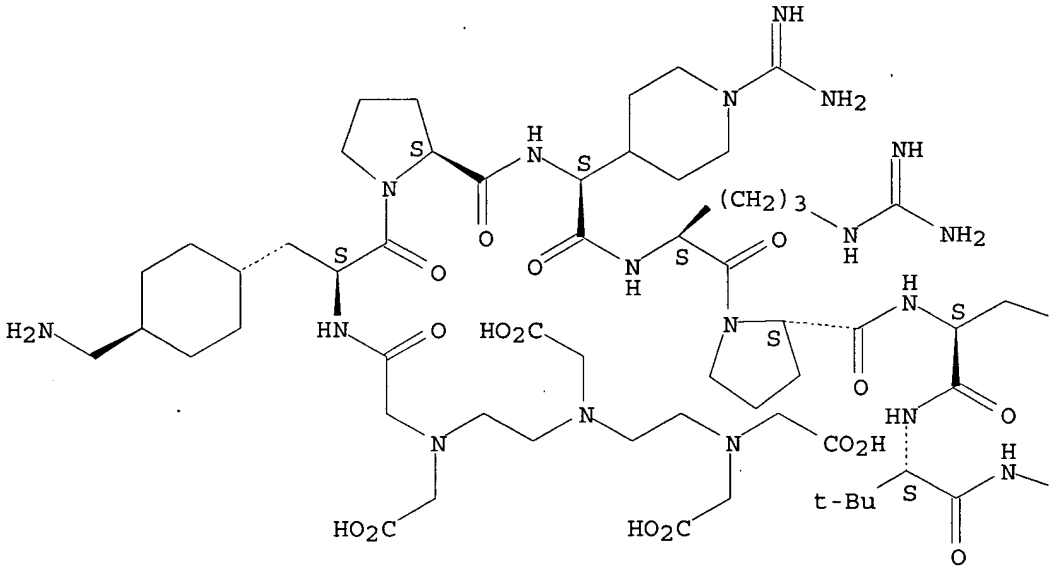

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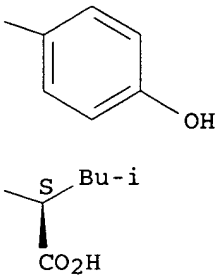

RN 578720-02-2 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-tyrosyl-L-α-glutamyl-L-asparaginyl-L-lysyl-L-prolyl-(2S)-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methyl-L-valyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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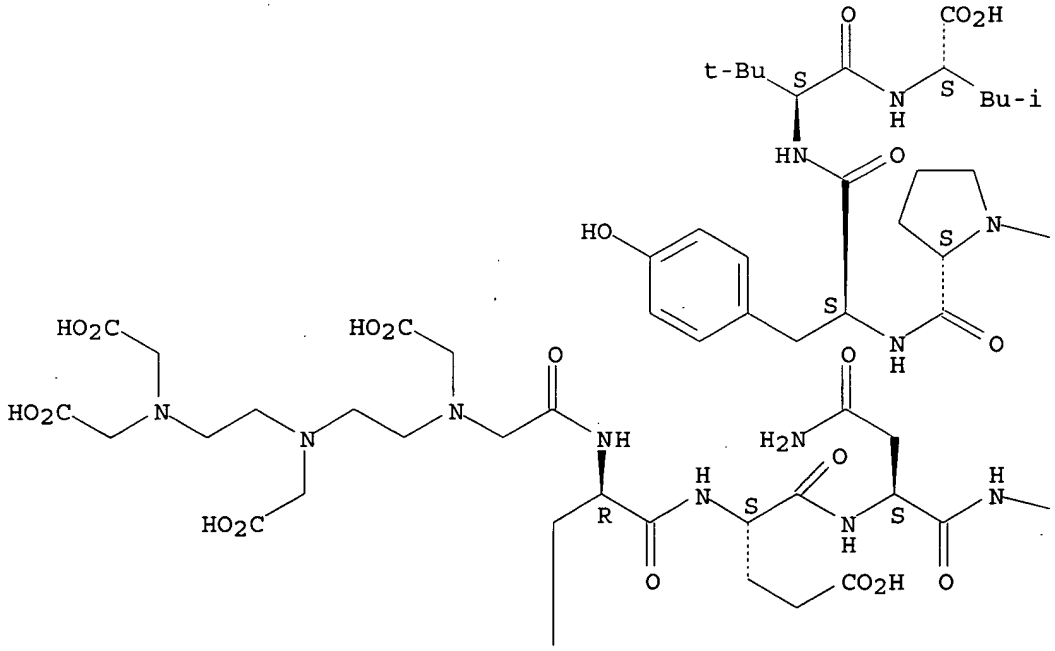

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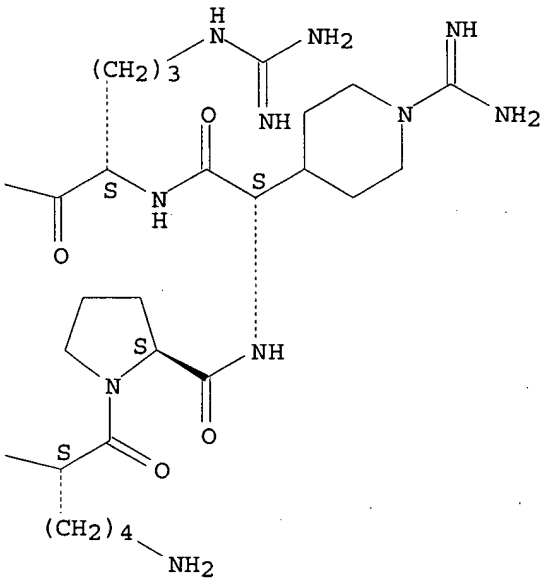

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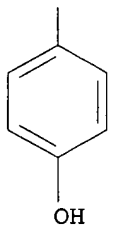

RN 578720-06-6 CAPLUS
CN L-Alanine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-(2S)-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methyl-L-valyl-3-cyclohexyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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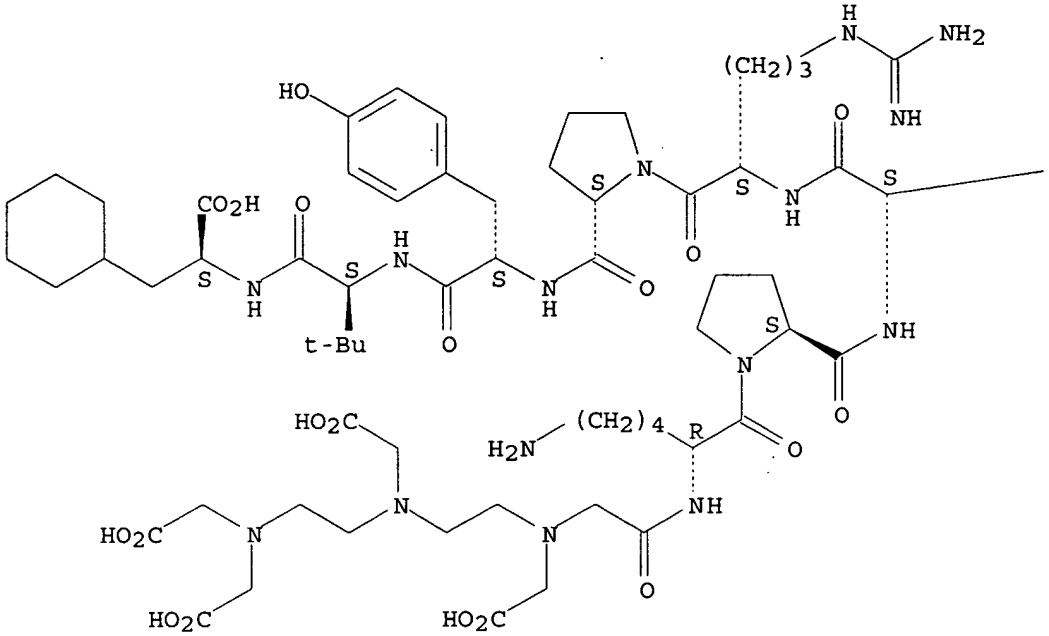

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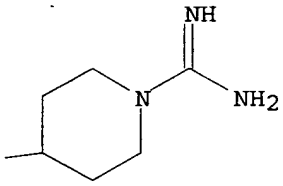

RN 578720-08-8 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-(2S)-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methyl-L-valyl-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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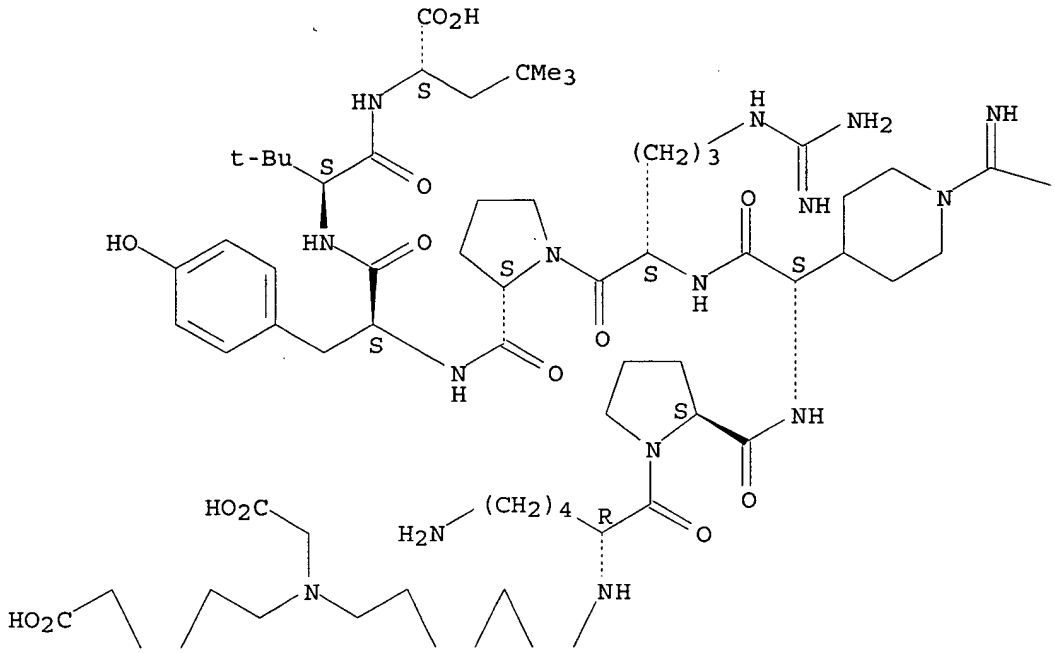

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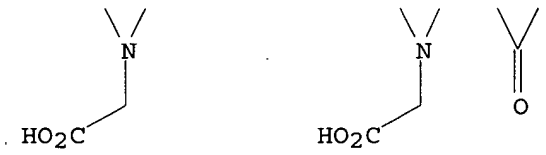

RN 578720-10-2 CAPLUS

CN L-Alanine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-tyrosyl-L-α-glutamyl-L-asparaginyl-L-lysyl-L-prolyl-(2S)-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methyl-L-valyl-3-cyclohexyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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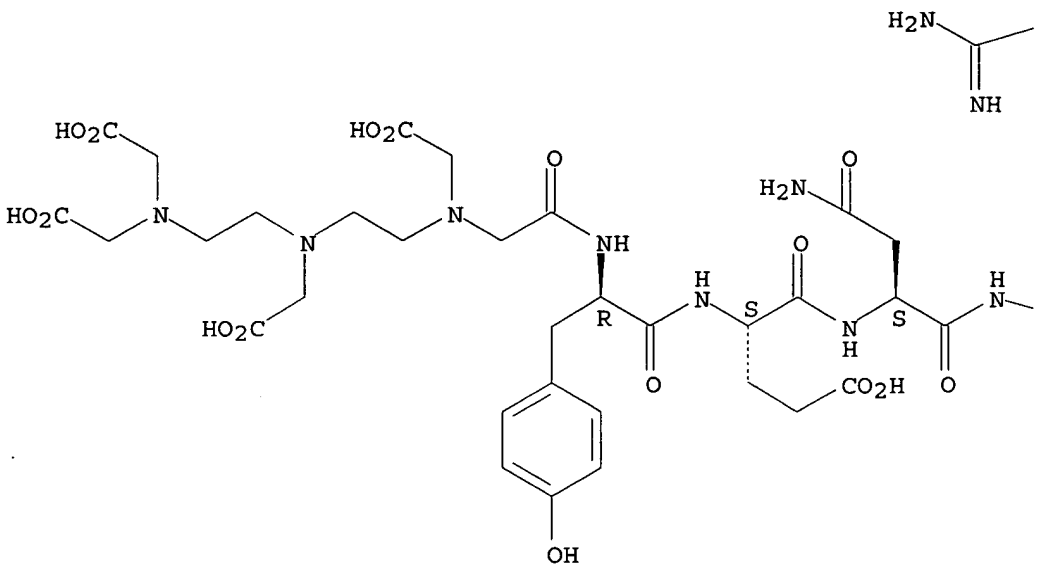

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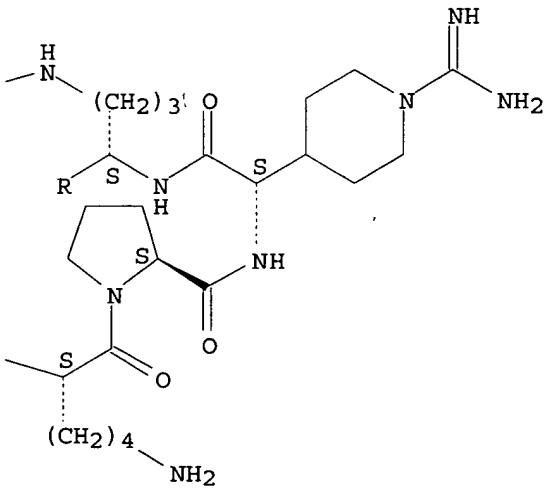

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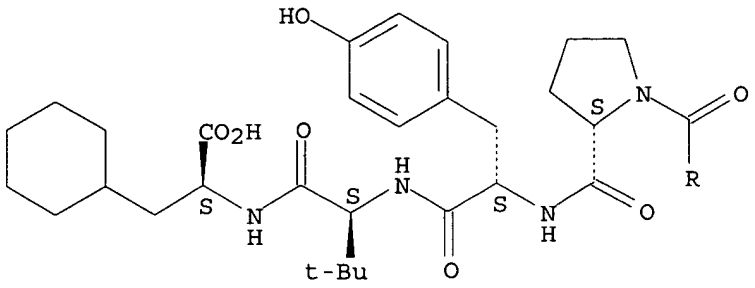

RN 578720-12-4 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-tyrosyl-L-α-glutamyl-L-asparaginyl-L-lysyl-L-prolyl-(2S)-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methyl-L-valyl-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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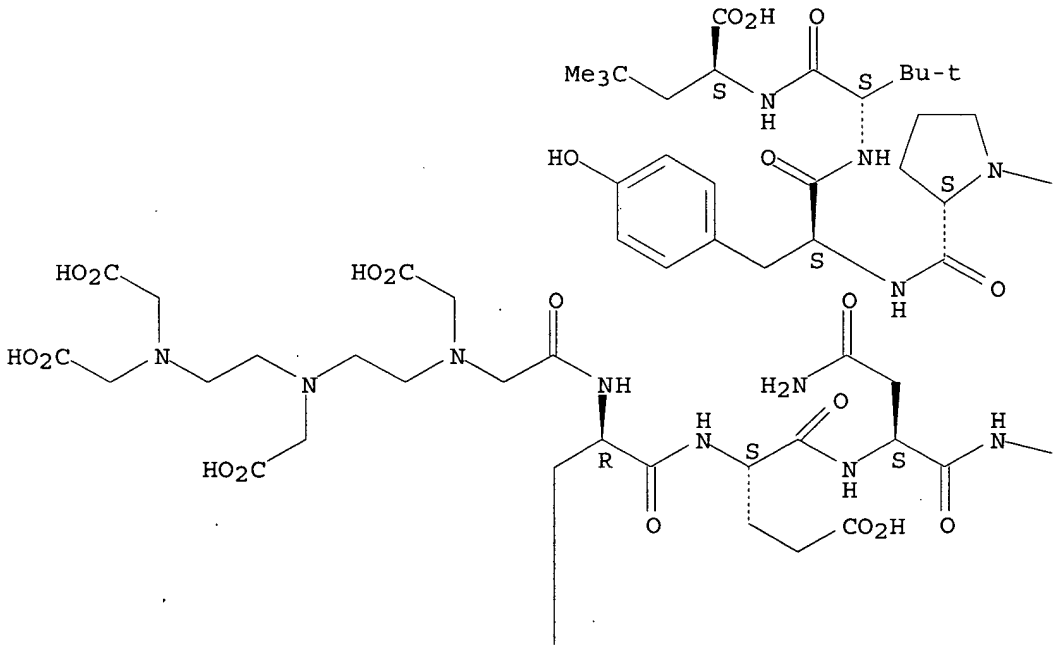

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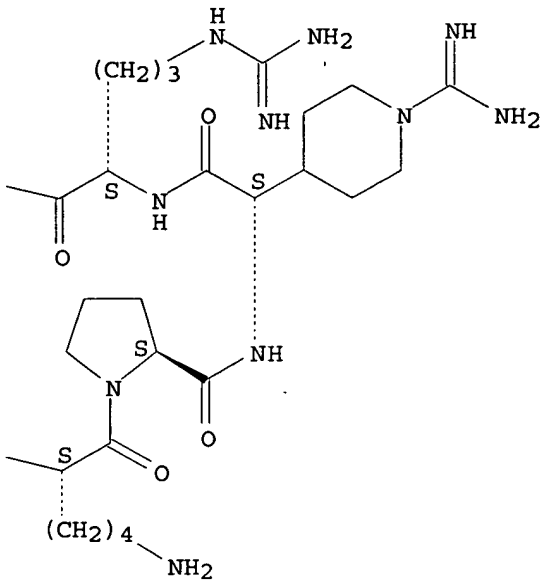

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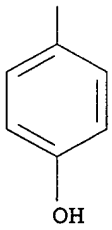

RN 579448-97-8 CAPLUS
CN 6-13-Neurotensin (cattle), 6-[N2-[[[3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5(or 6)-yl]amino]thioxomethyl]-D-lysine]-8-[(2S)-2-[1-(aminoiminomethyl)-4-piperidinyl]glycine]- (9CI) (CA INDEX NAME)

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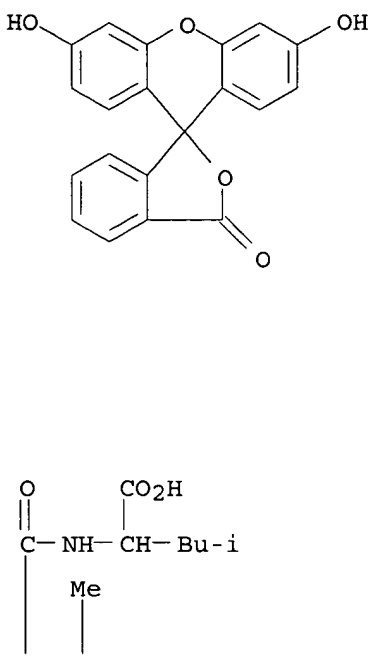

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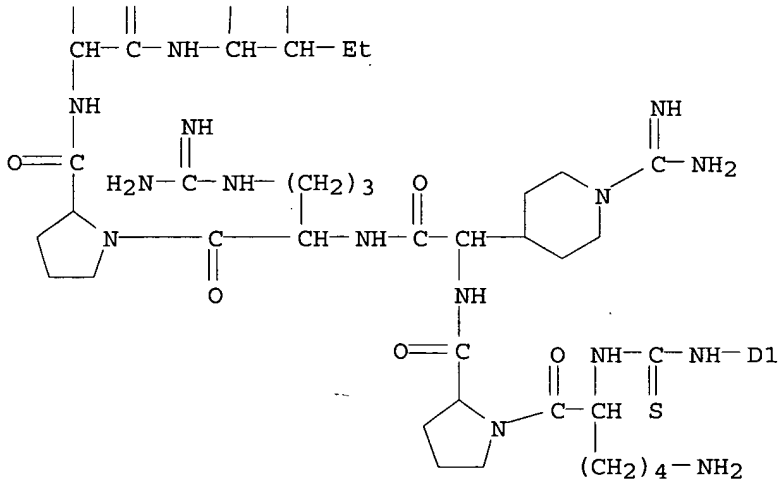

RN 579448-98-9 CAPLUS
CN 6-13-Neurotensin (cattle), 6-[N6-[[[3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5(or 6)-yl]amino]thioxomethyl]-D-lysine]-8-[(2S)-2-[1-(aminoiminomethyl)-4-piperidinyl]glycine]- (9CI) (CA INDEX NAME)

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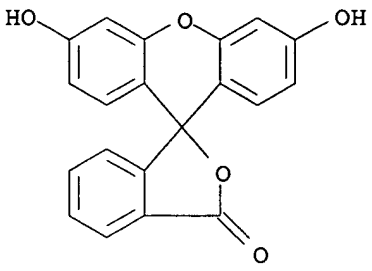

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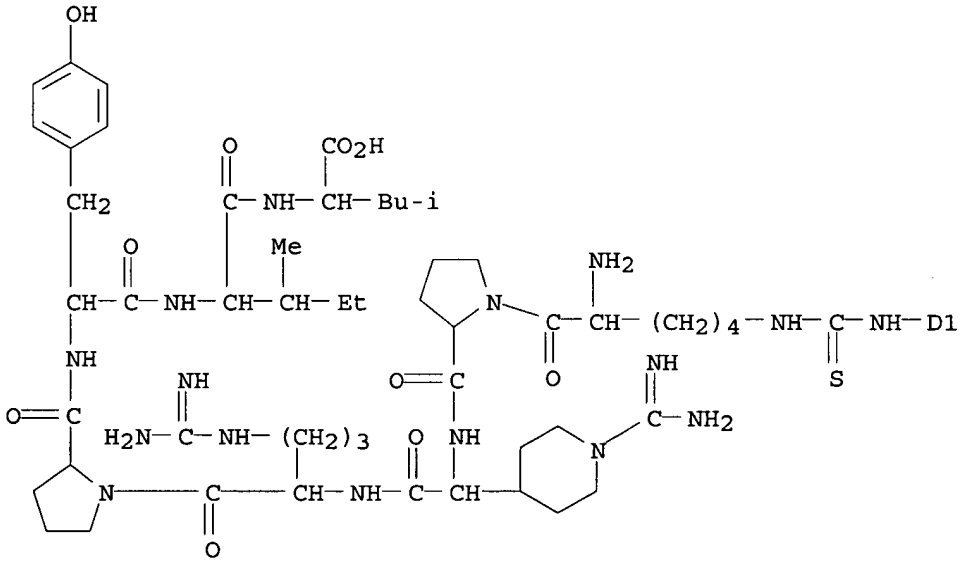

RN 579448-99-0 CAPLUS
CN 6-13-Neurotensin (cattle), 6-[N2,N6-bis[[[3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5(or 6)-yl]amino]thioxomethyl]-D-lysine]-8-[(2S)-2-[1-(aminoiminomethyl)-4-piperidinyl]glycine]- (9CI) (CA INDEX NAME)

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
RN 579449-00-6 CAPLUS
CN L-Leucine, (2S)-N-[[[3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5(or 6)-yl]amino]thioxomethyl]-2-(4-piperidinyl)glycyl-L-prolyl-(2S)-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methyl-L-valyl- (9CI) (CA INDEX NAME)

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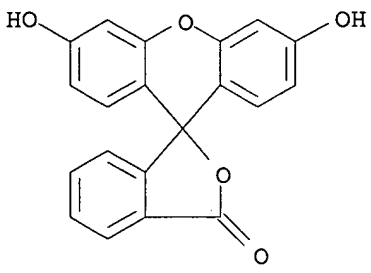

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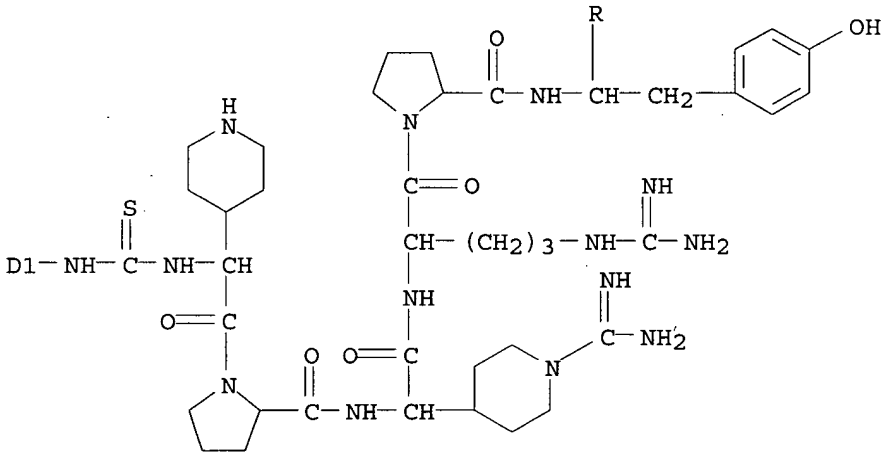

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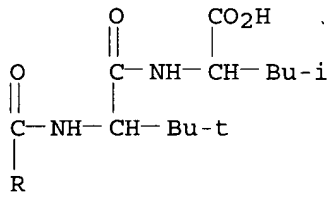

RN 579449-01-7 CAPLUS

CN L-Leucine, (2S)-2-[1-[[[3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5(or 6)-yl]amino]thioxomethyl]-4-piperidinyl]glycyl-L-prolyl-(2S)-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methyl-L-valyl- (9CI) (CA INDEX NAME)

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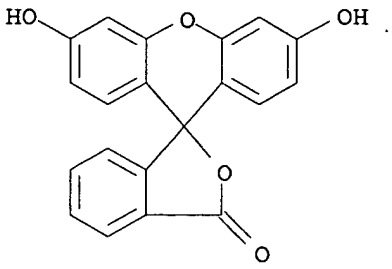

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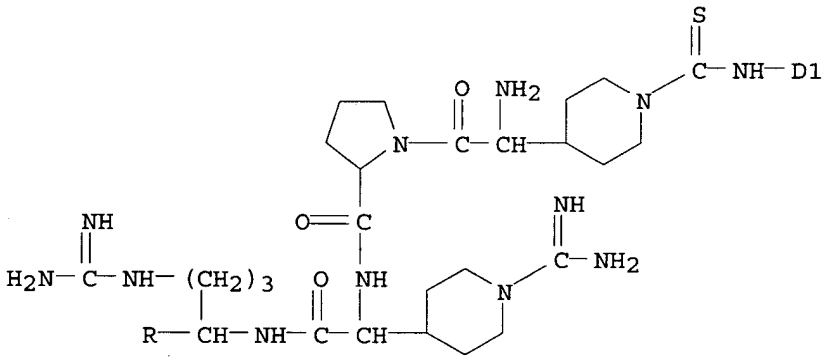
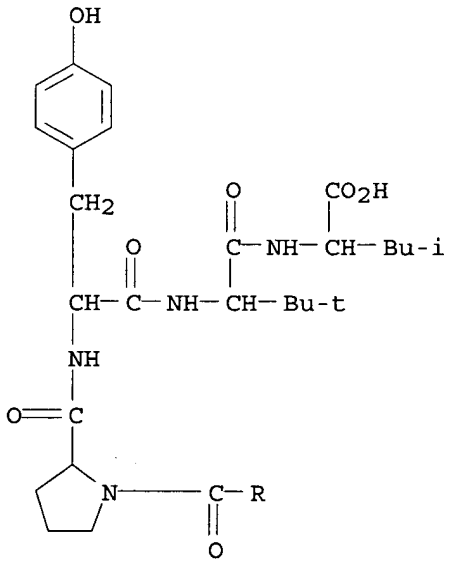


PAGE 3-A



RN 579449-02-8 CAPLUS
CN L-Leucine, (2S)-N-[[[3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5(or 6)-yl]amino]thioxomethyl]-2-[1-[[[3',6'-dihydroxy-3-

oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5(or 6)-yl]amino]thioxomethyl]-4-piperidinyl]glycyl-L-prolyl-(2S)-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methyl-L-valyl- (9CI) (CA INDEX NAME)

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

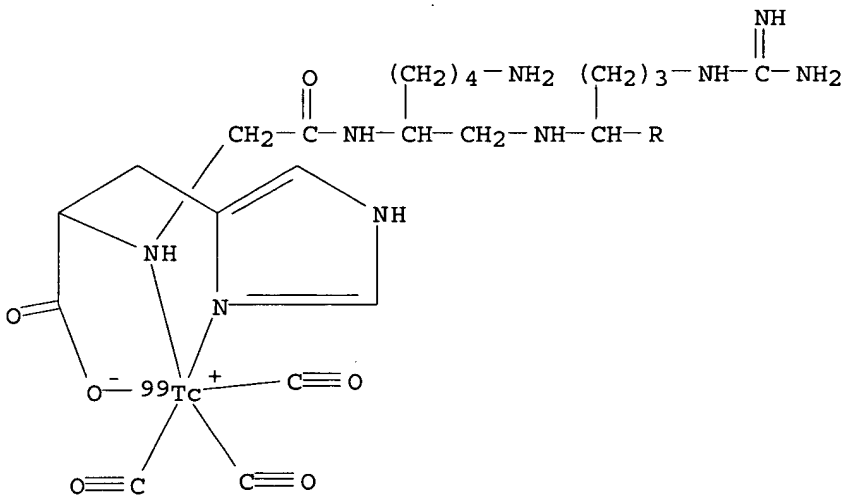
L45 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2005 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 2003:884747 CAPLUS
DOCUMENT NUMBER: 140:195456
TITLE: Radiolabeled neurotensin analog, 99mTc-NT-XI, evaluated in ductal pancreatic adenocarcinoma patients
AUTHOR(S): Buchegger, Franz; Bonvin, Florent; Kosinski, Marek; Schaffland, Andreas O.; Prior, John; Reubi, Jean C.; Blaeuenstein, Peter; Tourwe, Dirk; Garayoa, Elisa Garcia; Delaloye, Angelika Bischof
CORPORATE SOURCE: Division of Nuclear Medicine, University Hospital of Lausanne, Lausanne, Switz.
SOURCE: Journal of Nuclear Medicine (2003), 44(10), 1649-1654
CODEN: JNMEAQ; ISSN: 0161-5505
PUBLISHER: Society of Nuclear Medicine
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 Nov 2003
AB The study aim was to assess the safety, biodistribution, tissue kinetics, and tumor uptake of the 99mTc-labeled neurotensin (NT) analog NT-XI. Four patients presenting ductal pancreatic adenocarcinoma were studied with 99mTc-NT-XI. Patients were followed by scintigraphy up to 4 h and by continued blood and urinary sampling until surgery 18-22 h after injection. Surgical tissue samples were analyzed for radioactivity uptake and NT receptor expression. No side effects were observed on injection of 99mTc-NT-XI. Blood biol. half-lives α and β were 35 min (range, 17-62 min) and 230 min (range, 107-383 min), resp. Repeated whole-body scintigraphy performed in 2 patients showed a single exponential decrease of whole-body activity with half-lives of 101 and 232 min. Tracer elimination was mainly renal, with 92% and 98% of activity counted in urine in the first 20 h. Kidney, liver, spleen, and bone marrow activity uptake was observed in all patients. Tumor was not visualized in the first 3 patients but could be localized by tomoscintigraphy in the pancreas head region of patient 4. In vitro tissue anal. showed high expression of NT receptor in the tumor of patient 4, correlated with the highest tumor radioactivity uptake and the highest tumor-to-fat radioactivity ratio. In vitro receptor expression was also pos. in a second patient having a tumor characterized by very low cellularity; however, the remaining 2 tumors lacked NT receptor expression. Injection of 99mTc-NT-XI was well tolerated. The in vivo tumor uptake appeared specific as it was observed in the 1 patient with a pancreatic tumor that expressed high amts. of NT receptor. The results are compatible with preclin. animal results and in favor of further development of radiolabeled NT analogs for diagnosis or therapy of cancer.
IT **662112-41-6**

RL: ADV (Adverse effect, including toxicity); DGN (Diagnostic use); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(radiolabeled neurotensin analog 99mTc-NT-XI in ductal pancreatic adenocarcinoma patients)

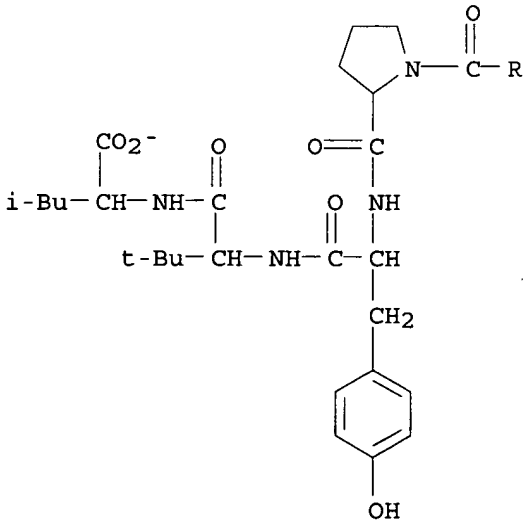
RN 662112-41-6 CAPLUS

CN Technetate(1-)-99Tc, [N-[(1S)-1-(carboxy-κO)-2-(1H-imidazol-4-yl-κN3)ethyl]glycyl-κN-L-lysyl-ψ(CH2-NH)-L-arginyl-L-prolyl-L-tyrosyl-3-methyl-L-valyl-L-leucinato(2-)]tricarbonyl-, hydrogen, (OC-6-44)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



PAGE 3-A

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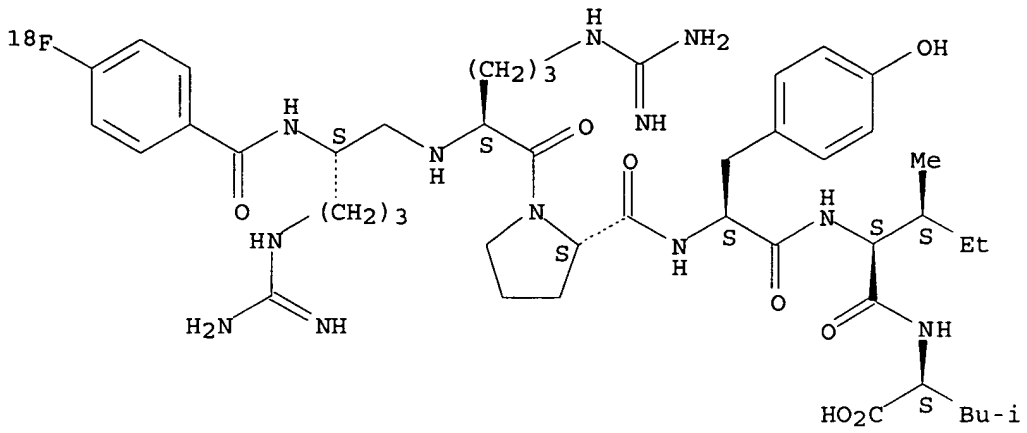
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

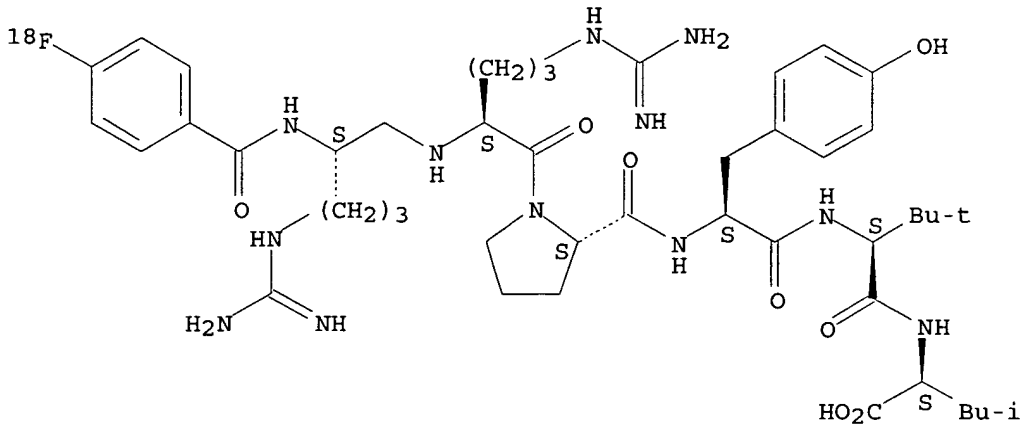
L45 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2005 ACS on STN DUPLICATE 3
ACCESSION NUMBER: 2002:23216 CAPLUS
DOCUMENT NUMBER: 136:275463
TITLE: Biodistribution and catabolism of 18F-labeled neurotensin(8-13) analogs
AUTHOR(S): Bergmann, Ralf; Scheunemann, Matthias; Heichert, Christoph; Mading, Peter; Wittrisch, Holm; Kretzschmar, Marion; Rodig, Heike; Tourwe, Dirk; Iterbeke, Koen; Chavatte, Kris; Zips, Daniel; Reubi, Jean Claude; Johannsen, Bernd
CORPORATE SOURCE: Institut fuer Bioanorganische und Radiopharmazeutische Chemie, Forschungszentrum Rossendorf, Germany
SOURCE: Nuclear Medicine and Biology (2002), 29(1), 61-72
CODEN: NMBIEO; ISSN: 0969-8051
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 10 Jan 2002
AB 4-([18F]fluoro)benzoyl-neurotensin(8-13) (18FB-Arg8-Arg9-Pro10-Tyr11-Ile12-Leu13-OH, 1) and two analogs stabilized in one and two positions (18FB-Arg8ψ(CH2NH)Arg9-Pro10-Tyr11- Ile12-Leu13-OH, 2, 18FB-Arg8ψ(CH2NH)Arg9-Pro10-Tyr11-Tle12-Leu13-OH, 3) were synthesized in a radiochem. yield of 25-36% and a specific activity of 5-15 GBq/mmol. The peptides were evaluated in vitro and in vivo for their potential to image tumors overexpressing neurotensin receptor 1 (NTR1) by positron emission tomog. (PET). All analogs exhibited in vitro binding affinity in the low nanomolar range to NTR1-expressing human tumors, measured by quant. receptor autoradiog., HT-29 and WiDr cells, and to sections of tumors derived from these cell lines in mice. The radiotracers were internalized in the cells in vitro, and the fluorinated peptides were able to mobilize intracellular Ca2+ of WiDr cells. In in vivo studies in rats and in mice bearing HT-29 cell tumors, only a moderate uptake of the radioligands into the studied tumors was observed, presumingly due to degradation in vivo and fast elimination by the kidneys. In comparison with the other analogs, the specific tumor uptake expressed as tumor-to-muscle relation was highest for the radioligand 3. The blood clearance of 3 was reduced by co-injection of peptidase inhibitors. The catabolic pathways of the radiofluorinated peptides were elucidated. The results suggest that the high binding affinity to NTR1 and the stabilization against proteolytic degradation are not yet sufficient for tumor imaging by PET.
IT **266352-47-0 406486-48-4**
RL: DGN (Diagnostic use); PKT (Pharmacokinetics); BIOL (Biological study); USES (Uses)
(biodistribution and catabolism of 18F-labeled neurotensin(8-13) analogs in relation to their potential to image tumors overexpressing neurotensin receptor 1 by PET)
RN 266352-47-0 CAPLUS
CN L-Leucine, N2-[(2S)-5-[(aminoiminomethyl)amino]-2-[[4-(fluoro-18F)benzoyl]amino]pentyl]-L-arginyl-L-prolyl-L-tyrosyl-L-isoleucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 406486-48-4 CAPLUS
CN L-Leucine, N2-[(2S)-5-[(aminoiminomethyl)amino]-2-[[4-(fluoro-18F)benzoyl]amino]pentyl]-L-arginyl-L-prolyl-L-tyrosyl-3-methyl-L-valyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L45 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2005 ACS on STN DUPLICATE 4
ACCESSION NUMBER: 2003:509728 CAPLUS
DOCUMENT NUMBER: 140:211244
TITLE: Serum-stable neurotensin analogs as potential imaging and therapeutic agents for pancreatic cancer
AUTHOR(S): Srinivasan, Ananth; Schmidt, Michelle A.; Erion, Jack L.; Bugaj, Joseph E.; Wilhelm, R. Randy; Webb, Elizabeth G.; Chinen, Lori K.; Reubi, Jean-Claude
CORPORATE SOURCE: Mallinckrodt, Inc., Hazelwood, MO, 63042, USA
SOURCE: Peptides 2000, Proceedings of the European Peptide Symposium, 26th, Montpellier, France, Sept. 10-15, 2000 (2001), Meeting Date 2000, 743-744. Editor(s): Martinez, Jean; Fehrentz, Jean-Alain. Editions EDK:

Paris, Fr.
CODEN: 69EDWK; ISBN: 2-84254-048-4
DOCUMENT TYPE: Conference
LANGUAGE: English
ED Entered STN: 04 Jul 2003

AB Novel neurotensin derivs. containing amino acid mimics were synthesized by replacing one or both arginines by its mimic. Replacement of Arg8 by Gly(piperidinylamidino) [Gly(PipAm)] resulted in retention of the binding affinity while increasing the serum stability. Addnl. analogs were prepared by substituting Lys6 with constrained lysines [glycine(piperidinyl) [Gly(Pip)] and trans-(aminomethyl)cyclohexylalanine (tr-(4-CH2NH2-Cha))] and leucine12 with cyclohexylalanine (Cha) or t-butyl-alanine. All of these compds. contain DTPA at the N-terminus for the incorporation of In-111 for γ-ray scintigraphy. The binding affinities were measured using frozen tissue sections from receptor-sensitive human tumors and compared against radioiodinated natural neurotensin. The results for the compound containing the sequence DTPA-Gly(Pip)-P-Gly(PipAm)-R-P-Y-tBuGly-L-OH indicated that the tumor uptake is specific and the label is retained in the tumor. Thus, this compound is an ideal agent for the imaging and therapy of exocrine pancreatic cancer.

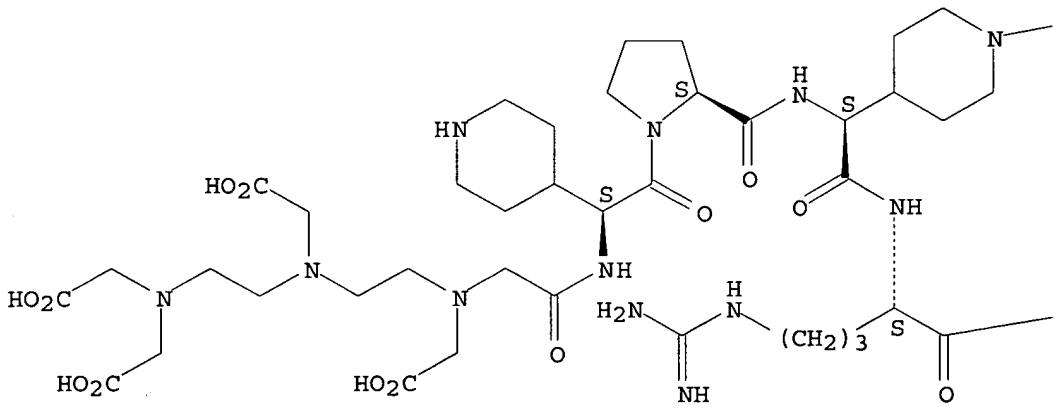
IT **578719-98-9P 578720-00-0P 578720-02-2P 578720-10-2P 578720-12-4P 664334-81-0P**
RL: BPN (Biosynthetic preparation); BSU (Biological study, unclassified); PAC (Pharmacological activity); PKT (Pharmacokinetics); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(serum-stable neurotensin analogs as potential imaging and therapeutic agents for pancreatic cancer)

RN 578719-98-9 CAPLUS

CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-(2S)-2-(4-piperidinyl)glycyl-L-prolyl-(2S)-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methyl-L-valyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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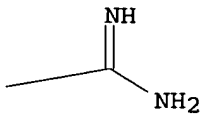

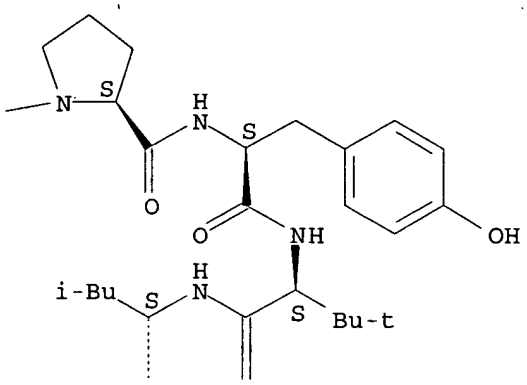

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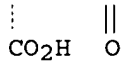
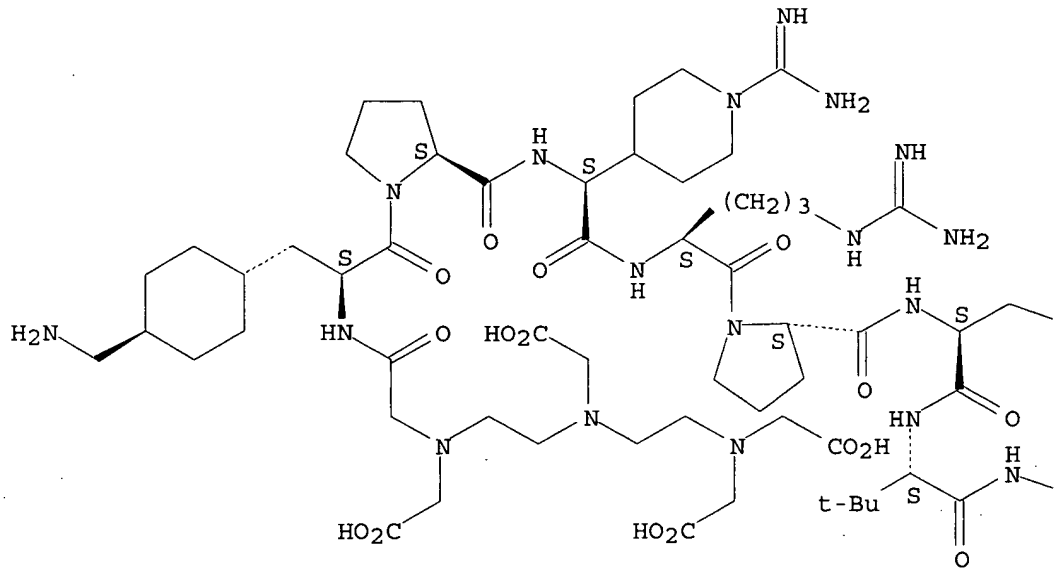


RN 578720-00-0 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-3-[trans-4-(aminomethyl)cyclohexyl]-L-alanyl-L-prolyl-(2S)-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methyl-L-valyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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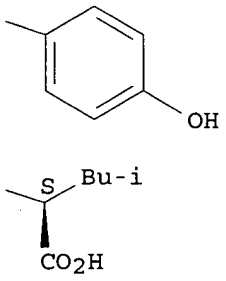
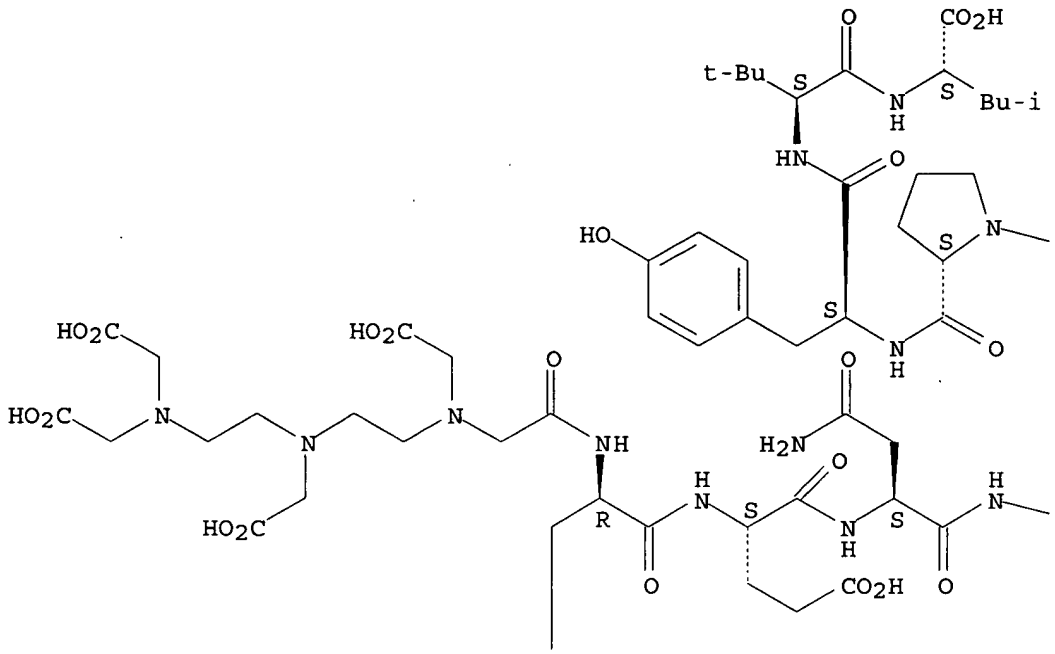


RN 578720-02-2 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-tyrosyl-L-α-glutamyl-L-asparaginyl-L-lysyl-L-prolyl-(2S)-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methyl-L-valyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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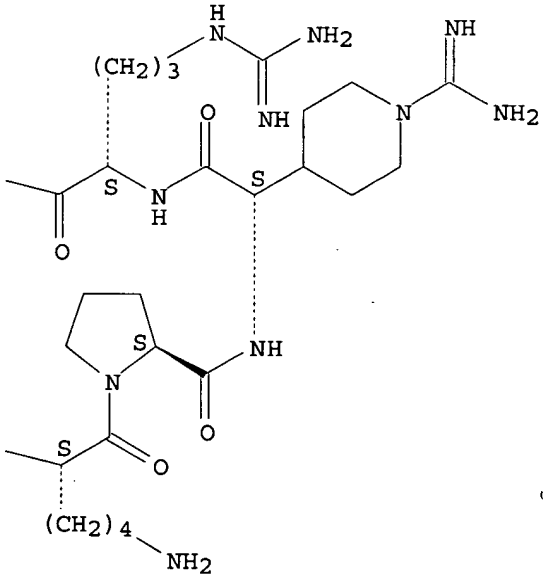

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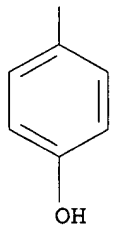

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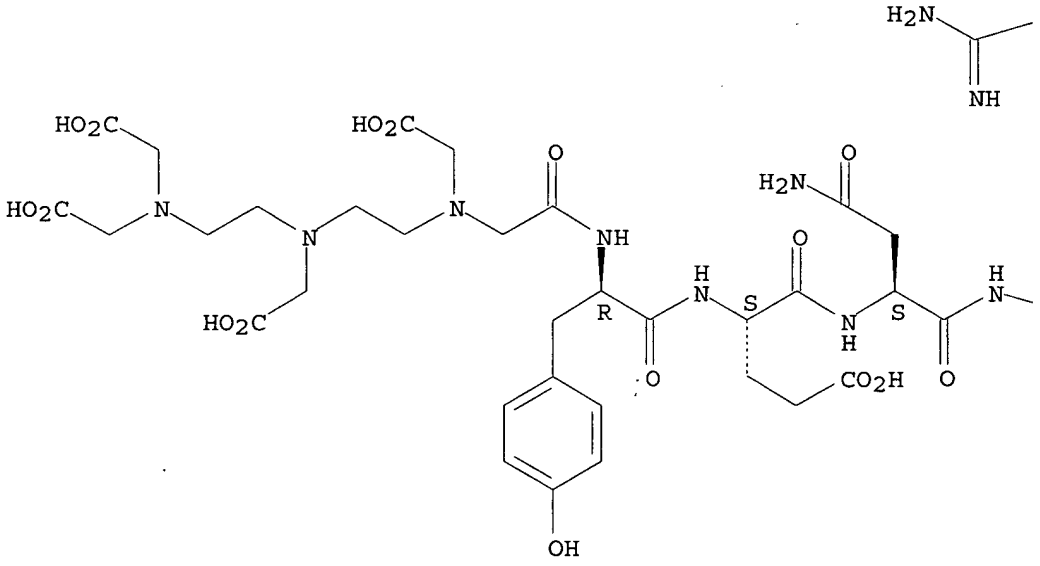
Absolute stereochemistry.

PAGE 1-A



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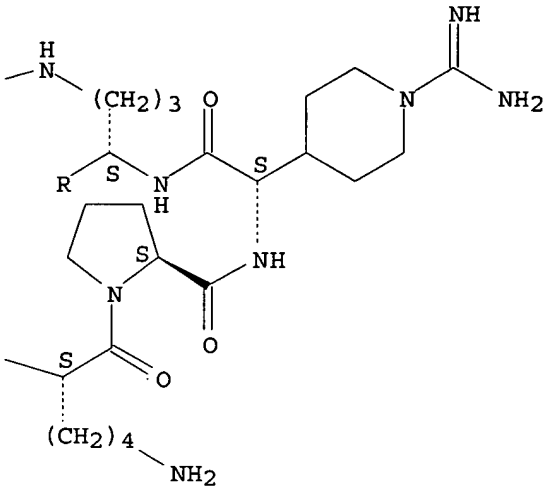

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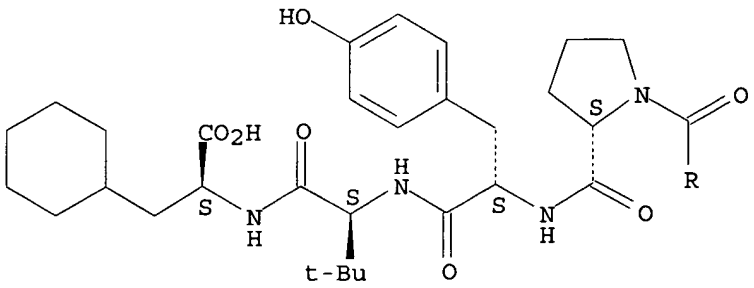

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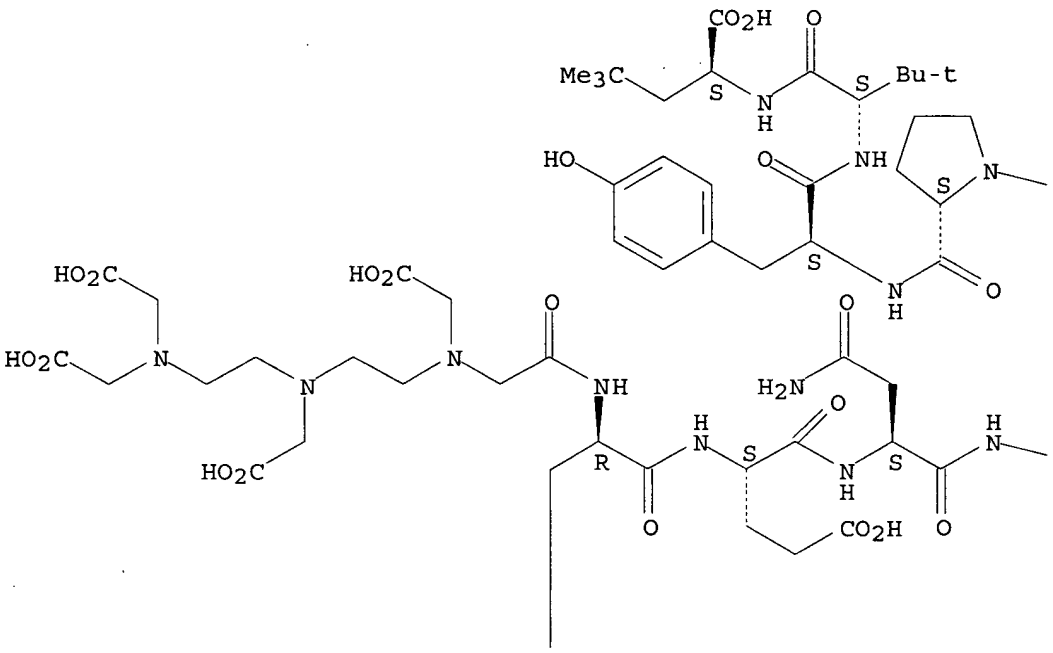
Absolute stereochemistry.

PAGE 1-A



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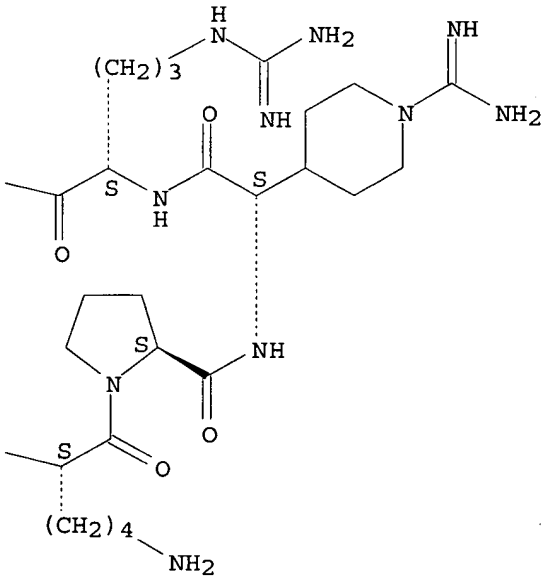

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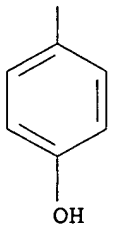
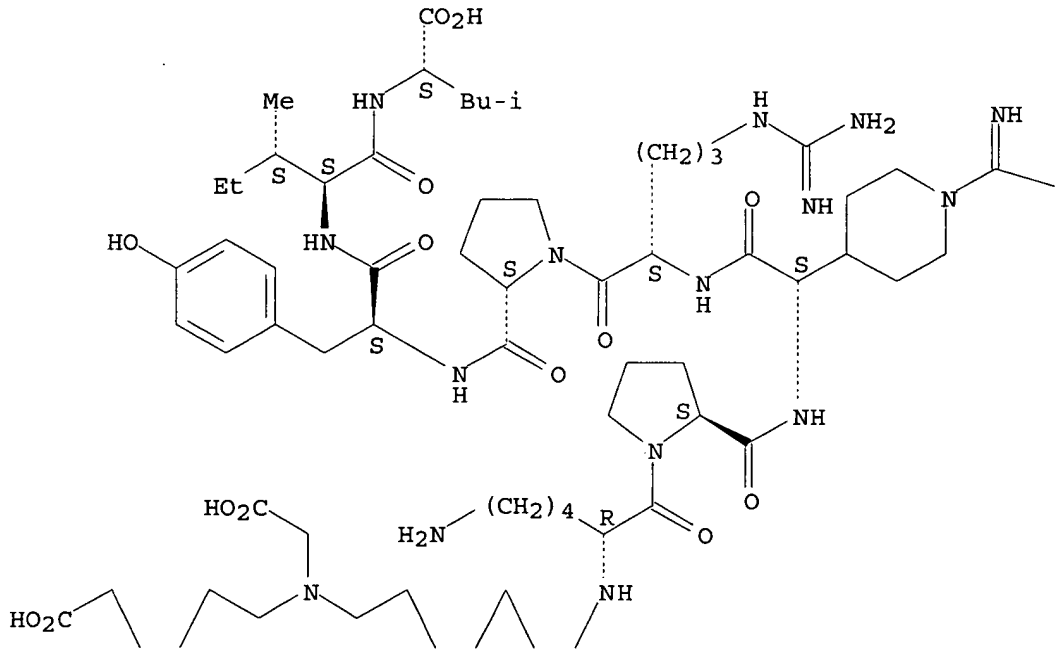


RN 664334-81-0 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-(2S)-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-L-isoleucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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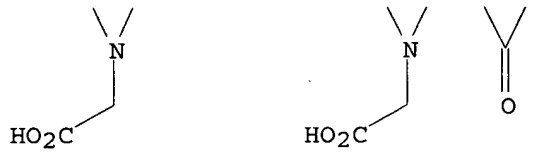
PAGE 2-A



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L45 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2005 ACS on STN DUPLICATE 5
ACCESSION NUMBER: 2000:911287 CAPLUS
DOCUMENT NUMBER: 134:76371
TITLE: Labeled neurotensin derivatives
INVENTOR(S): Srinivasan, Ananthachari; Erion, Jack L.; Schmidt, Michelle A.
PATENT ASSIGNEE(S): Mallinckrodt Inc., USA
SOURCE: PCT Int. Appl., 38 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000078796	A2	20001228	WO 2000-US17509	20000622
WO 2000078796	A3	20010517		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2374270	AA	20001228	CA 2000-2374270	20000622
EP 1194444	A2	20020410	EP 2000-950253	20000622
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				

PRIORITY APPLN. INFO.:

US 1999-140913P	P	19990624
US 2000-213068P	P	20000621
WO 2000-US17509	W	20000622

OTHER SOURCE(S): MARPAT 134:76371
ED Entered STN: 29 Dec 2000
AB Peptide analogs of neurotensin containing Arg mimics were synthesized which are resistant to enzymic degradation and which retain high binding affinity for neurotensin receptors. Best results in terms of serum stability are obtained by replacing the Arg8 with (4-Glu)Phe or (N-amidinopiperidinyl)glycine as the arginine surrogate. Another source of instability is the C-terminus with the Ile-Leu-OH being metabolized. Replacement of the C-terminus with a bulkier side chain stabilizes the bond from degradation Replacement of Ile with tBuGly results in no loss of binding affinity. Radiolabeled pharmaceutical compns. of these compds. are useful for diagnosis and therapy of tumors containing neurotensin receptors.

IT **314270-07-0 314270-07-0D**, indium-111 complex
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314270-11-6 314270-11-6D, indium-111 complex
314270-13-8 314270-14-9 314270-18-3
314270-20-7 314270-24-1 314270-32-1
314270-32-1D, indium-111 complex **314270-34-3**
314270-34-3D, indium-111 complex **314270-38-7**
314270-43-4 314270-46-7 314270-47-8
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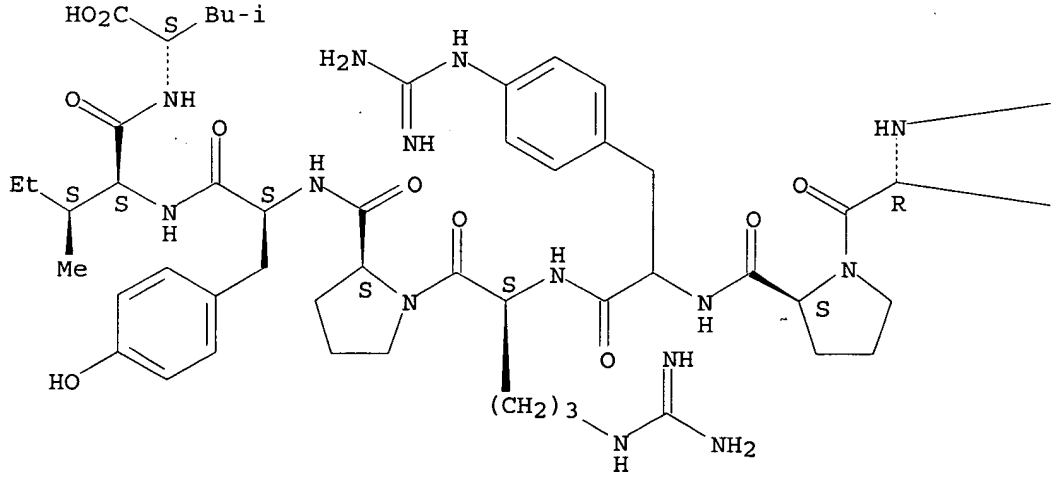
314295-72-2 314295-74-4 314295-75-5
314295-76-6
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(neurotensin analogs with increased serum and urine stability and receptor binding affinity)

RN 314270-07-0 CAPLUS

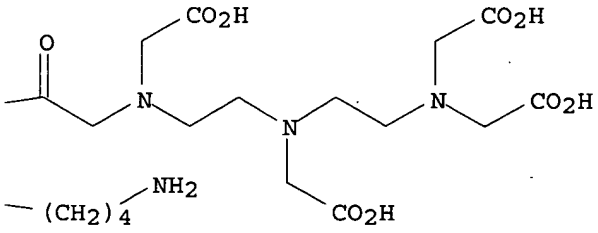
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-4-[(aminoiminomethyl)amino]phenylalanyl-L-arginyl-L-prolyl-L-tyrosyl-L-isoleucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



RN 314270-07-0 CAPLUS
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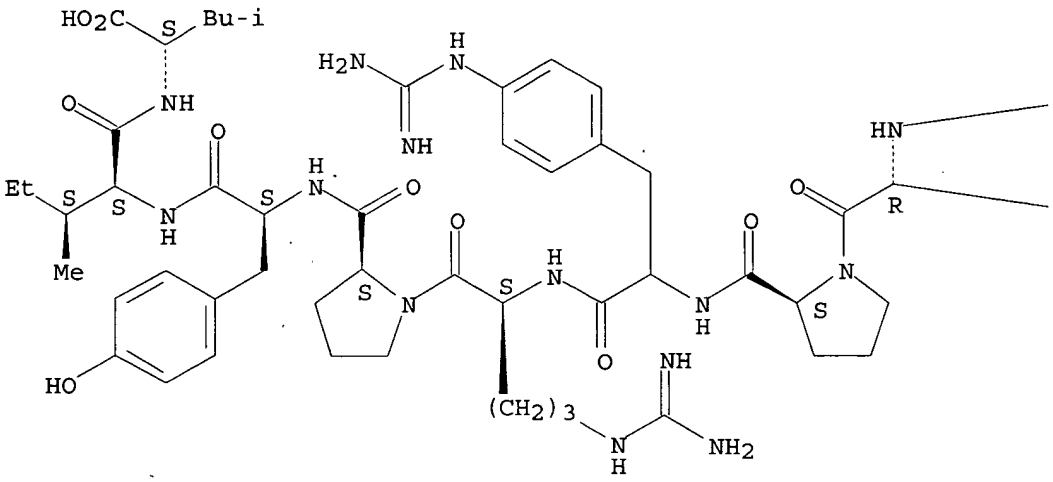
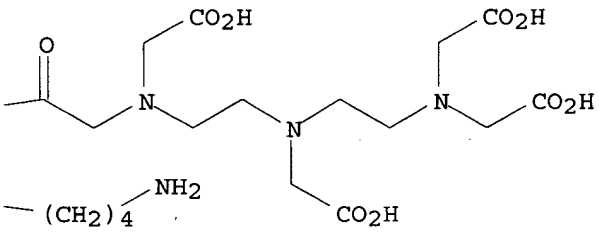
Absolute stereochemistry.

PAGE 1-A



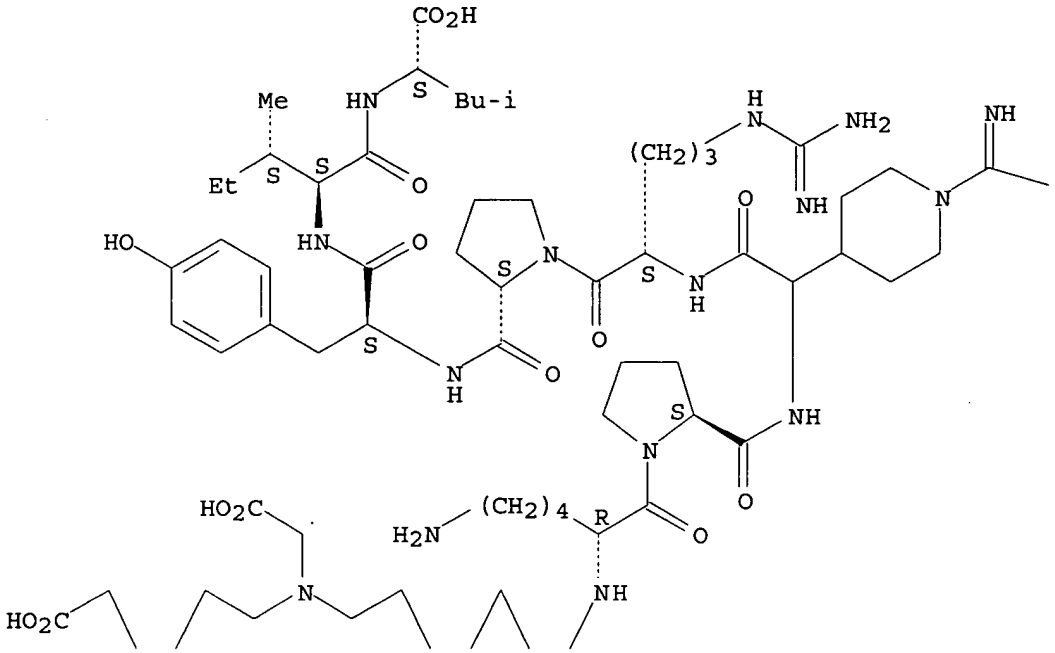
PAGE 1-B



RN 314270-09-2 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-L-isoleucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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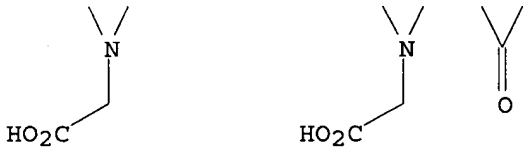
PAGE 2-A

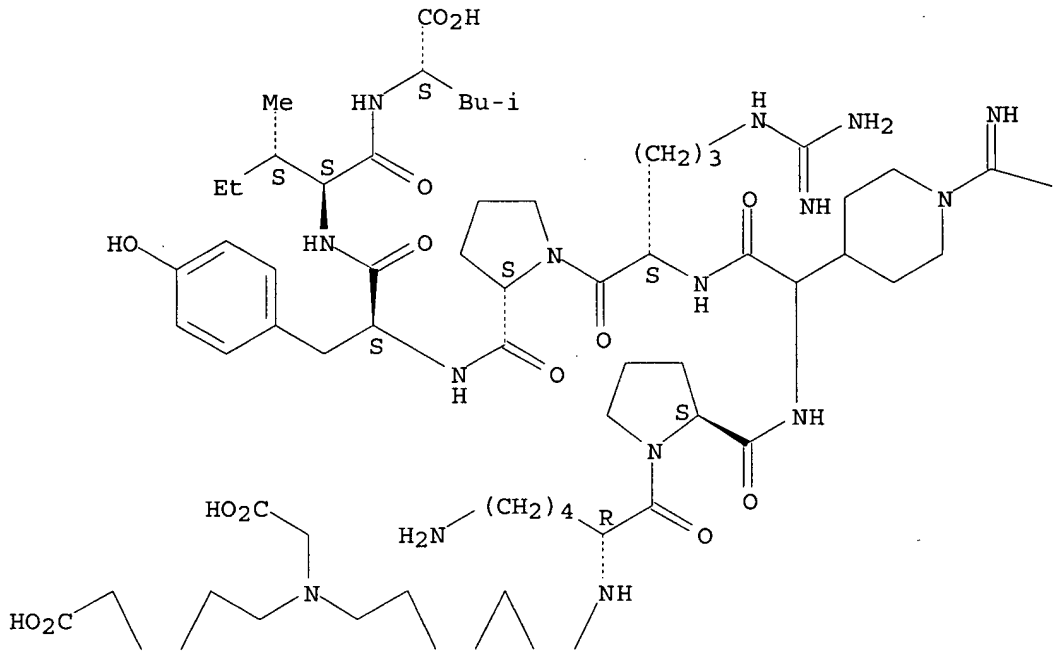


RN 314270-09-2 CAPLUS

CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-L-isoleucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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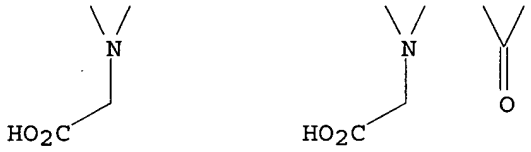
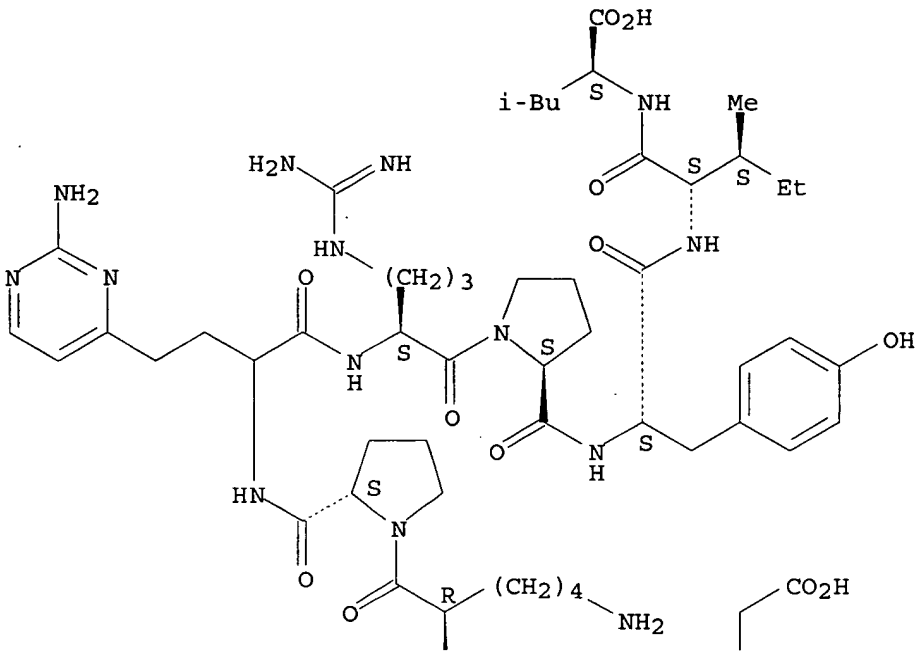
PAGE 2-A



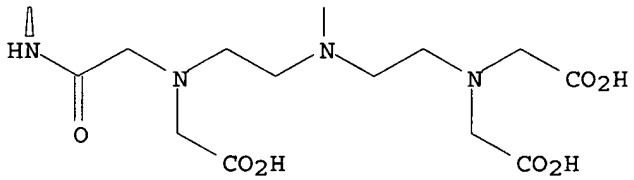
RN 314270-11-6 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-α,2-diamino-4-pyrimidinebutanoyl-L-arginyl-L-prolyl-L-tyrosyl-L-isoleucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



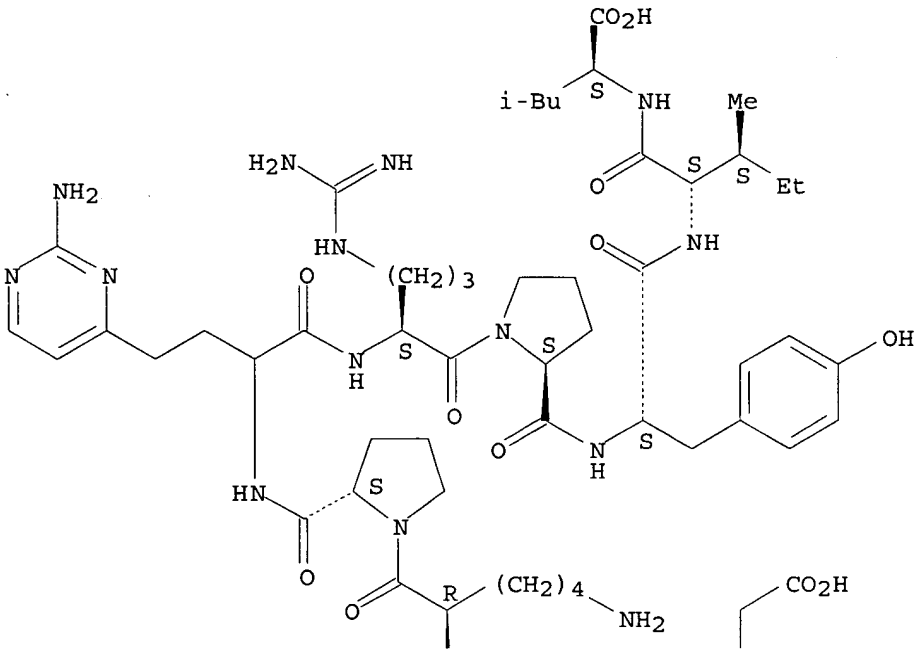
PAGE 2-A



RN 314270-11-6 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-α,2-diamino-4-pyrimidinebutanoyl-L-arginyl-L-prolyl-L-tyrosyl-L-isoleucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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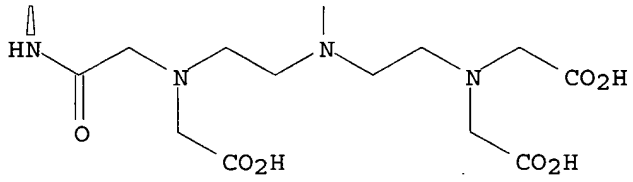
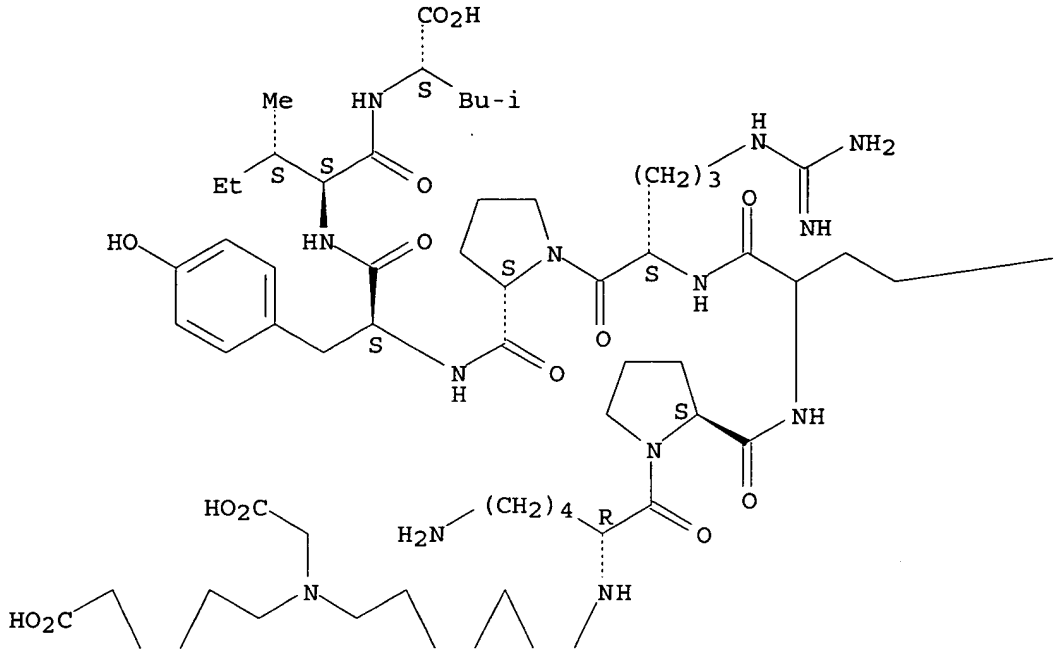


RN 314270-13-8 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-α-amino-1-(aminoiminomethyl)-4-piperidinebutanoyl-L-arginyl-L-prolyl-L-tyrosyl-L-isoleucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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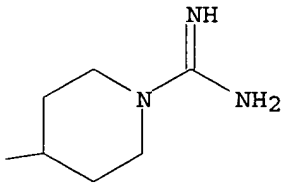

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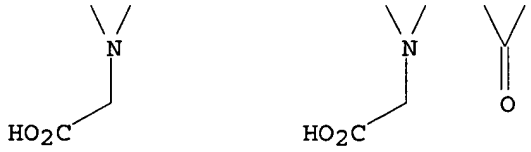
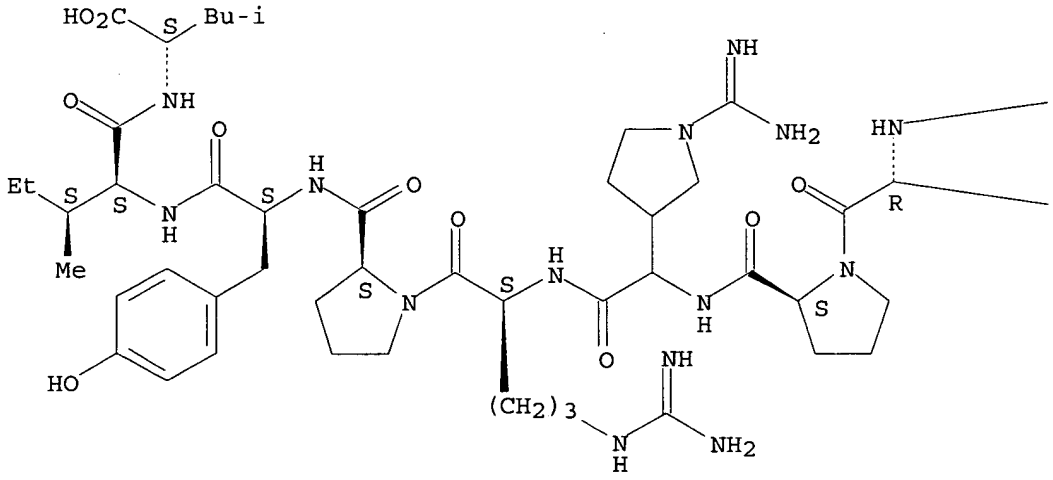


RN 314270-14-9 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-2-[1-(aminoiminomethyl)-3-pyrrolidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-L-isoleucyl- (9CI) (CA INDEX NAME)

Searched by Barb O'Bryen, STIC 2-2518

Absolute stereochemistry.

PAGE 1-A



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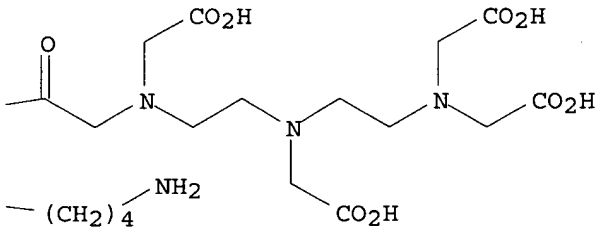

RN 314270-18-3 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-3-[1-(aminoiminomethyl)-3-pyrrolidinyl]alanyl-L-arginyl-L-prolyl-L-tyrosyl-L-isoleucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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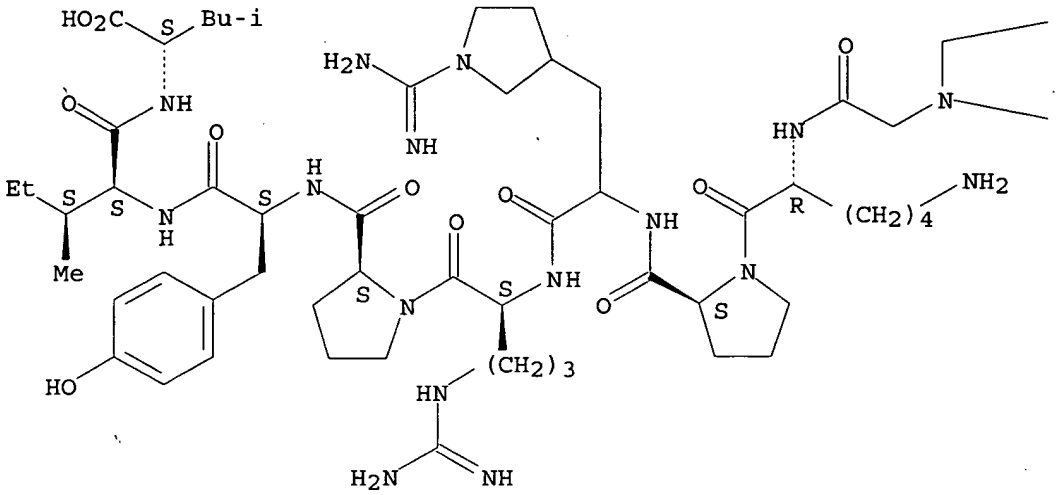

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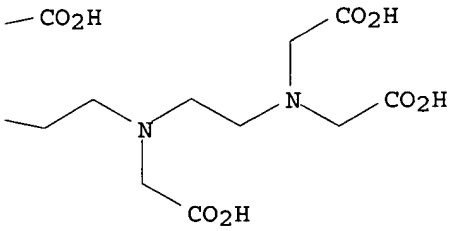

RN 314270-20-7 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-4-[(aminoiminomethyl)amino]phenylalanyl-4-[(aminoiminomethyl)amino]phenylalanyl-L-prolyl-L-tyrosyl-L-isoleucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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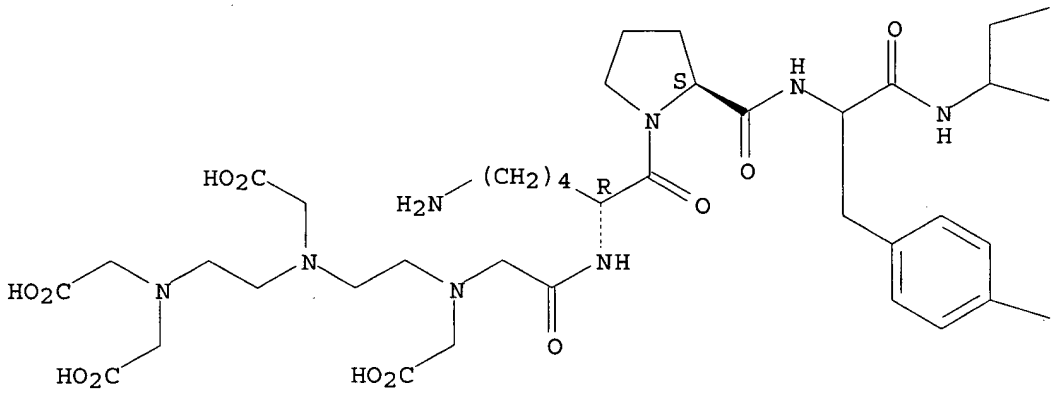

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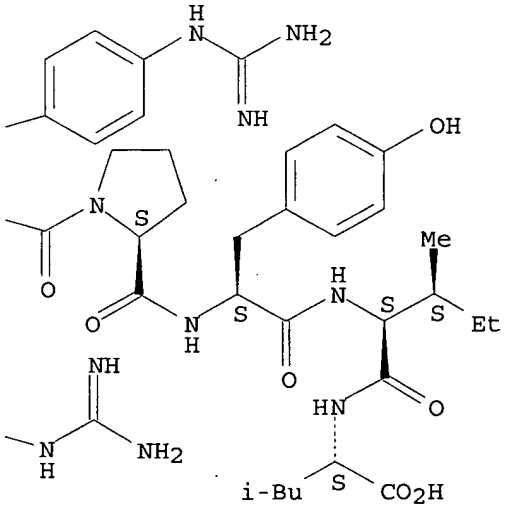

RN 314270-24-1 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-α,2-diamino-4-pyrimidinebutanoyl-α,2-diamino-4-pyrimidinebutanoyl-L-prolyl-L-tyrosyl-L-isoleucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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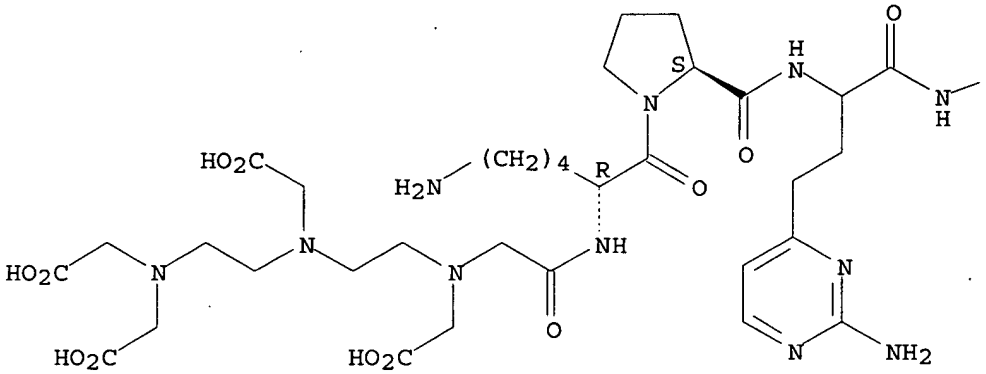

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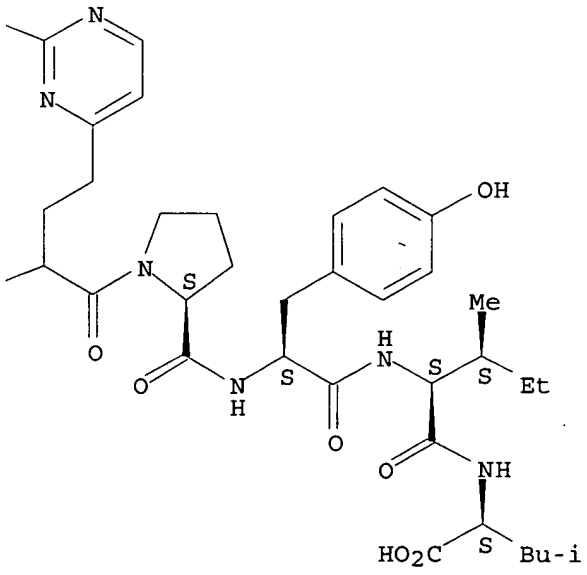

RN 314270-32-1 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-4-[(aminoiminomethyl)amino]phenylalanyl-L-arginyl-L-prolyl-L-tyrosyl-3-methylvalyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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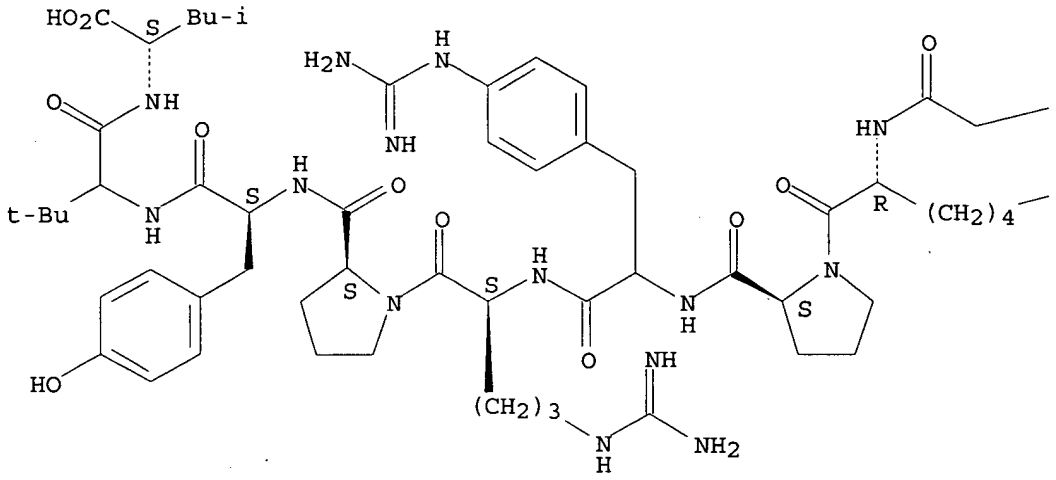

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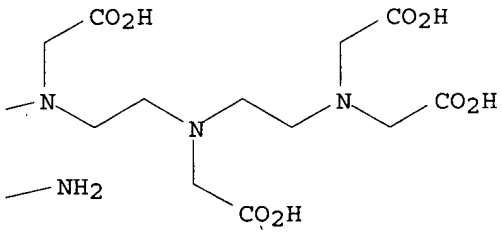
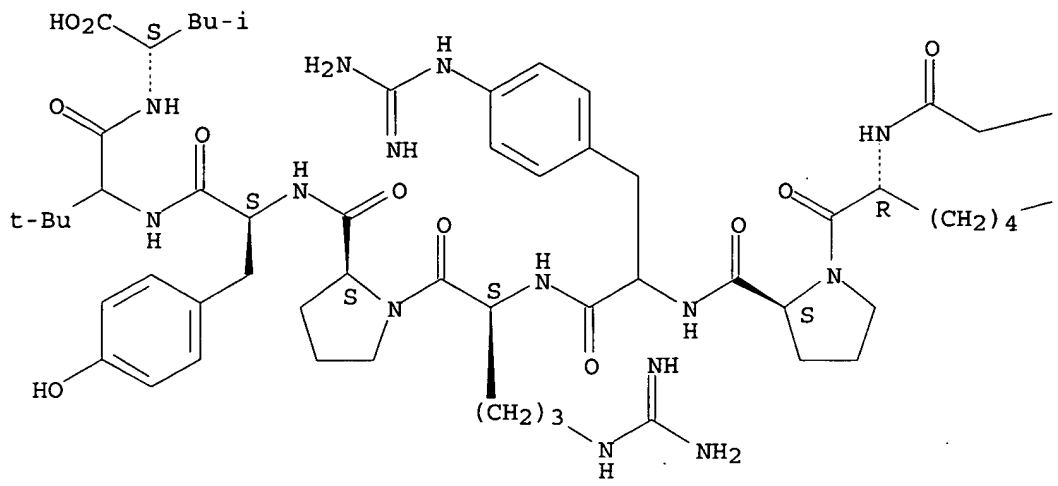


RN 314270-32-1 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-4-[(aminoiminomethyl)amino]phenylalanyl-L-arginyl-L-prolyl-L-tyrosyl-3-methylvalyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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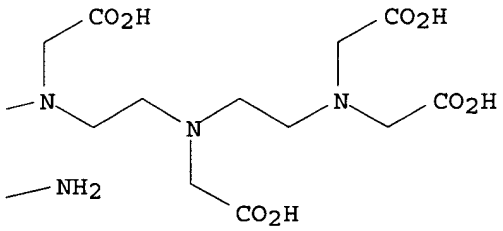
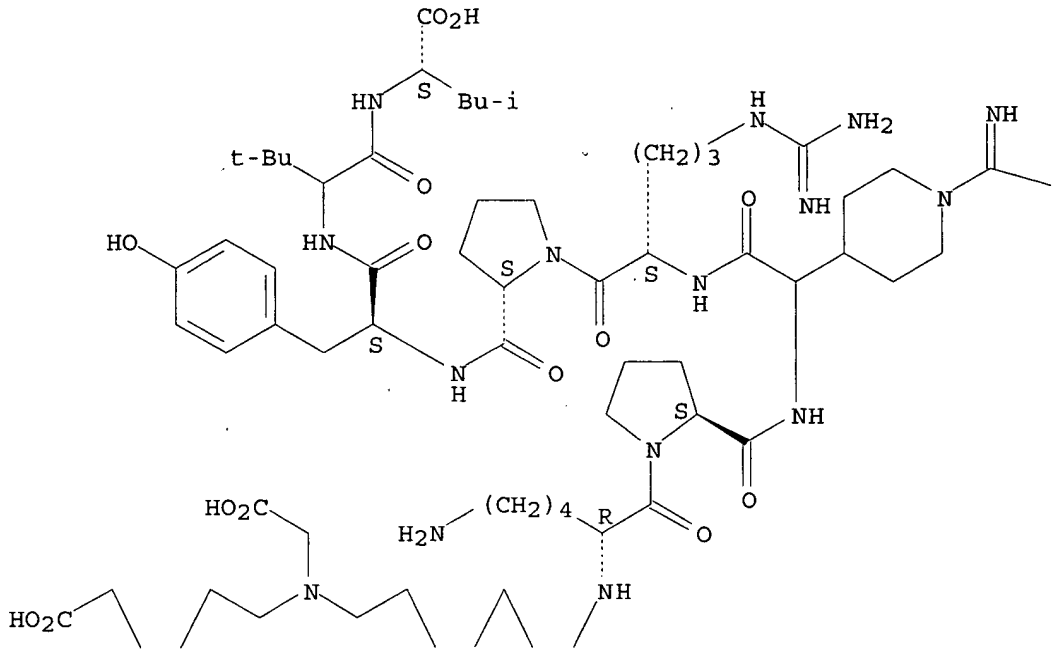


RN 314270-34-3 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methylvalyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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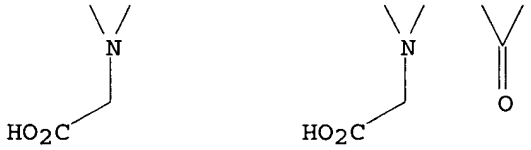
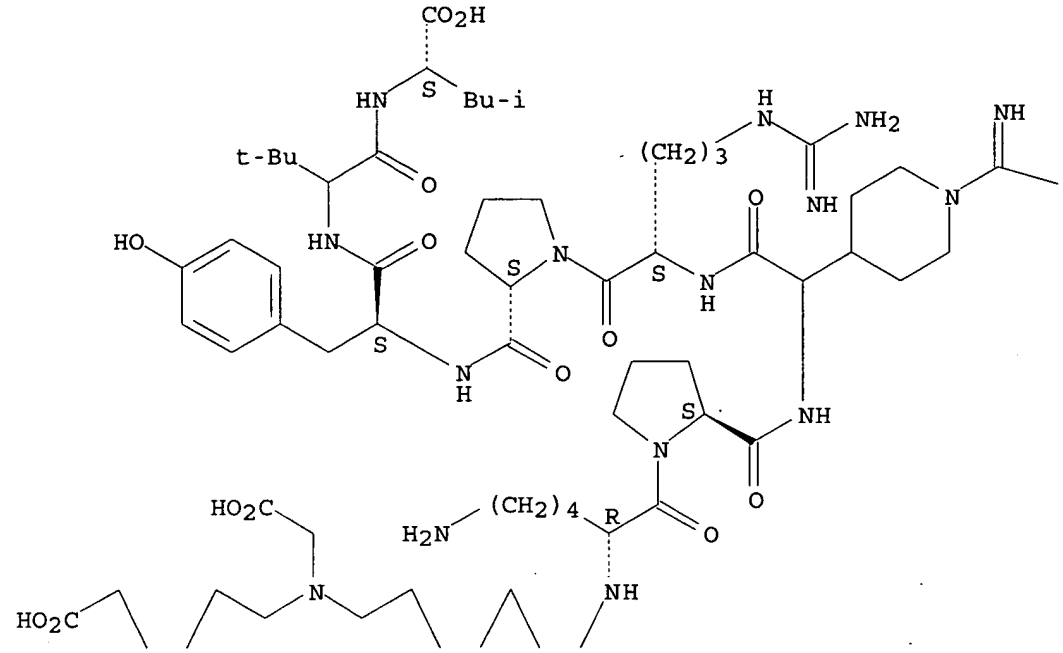


RN 314270-34-3 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methylvalyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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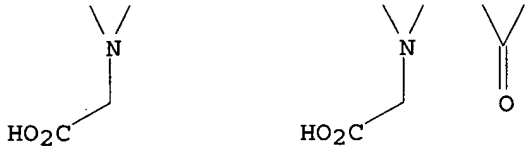
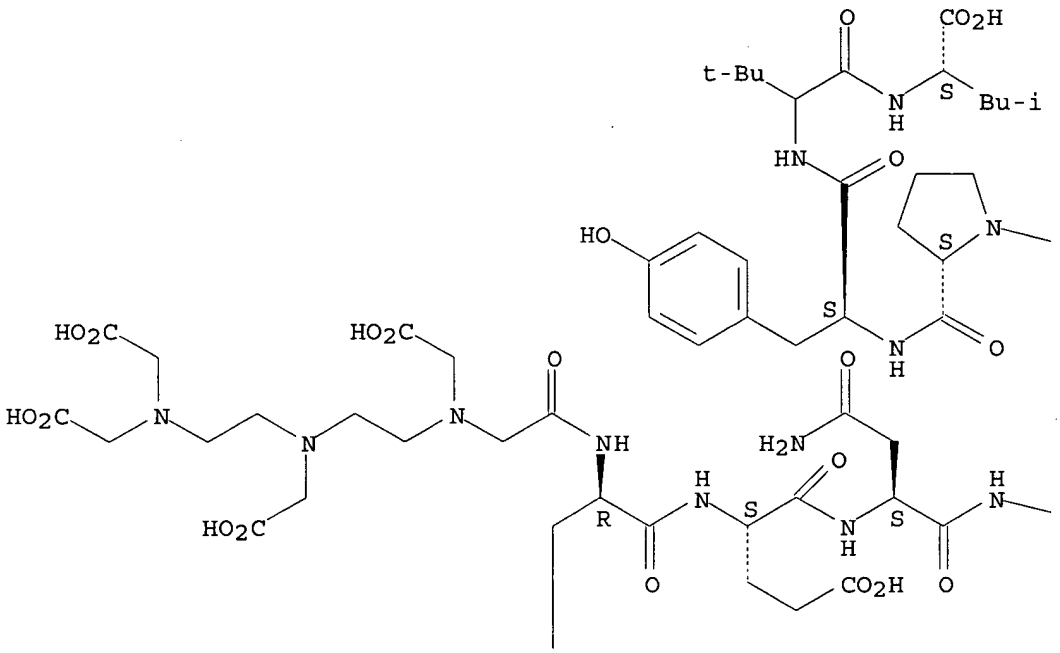


RN 314270-38-7 CAPLUS

CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-tyrosyl-L-α-glutamyl-L-asparaginyl-L-lysyl-L-prolyl-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methylvalyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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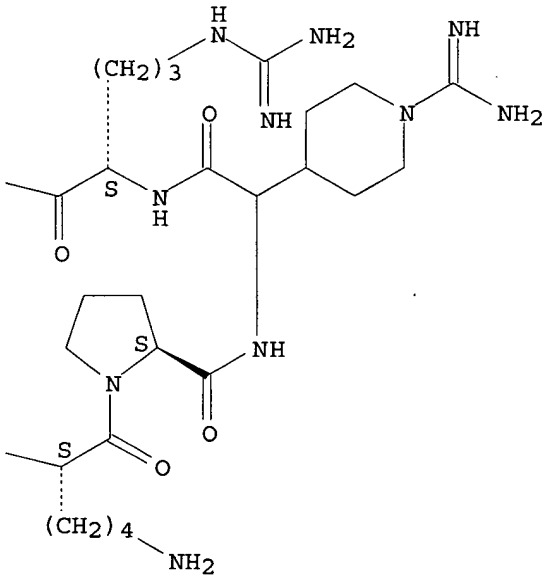

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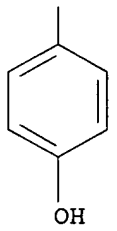

RN 314270-43-4 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-4-oxo-D-prolyl-L-tyrosyl-3-methylvalyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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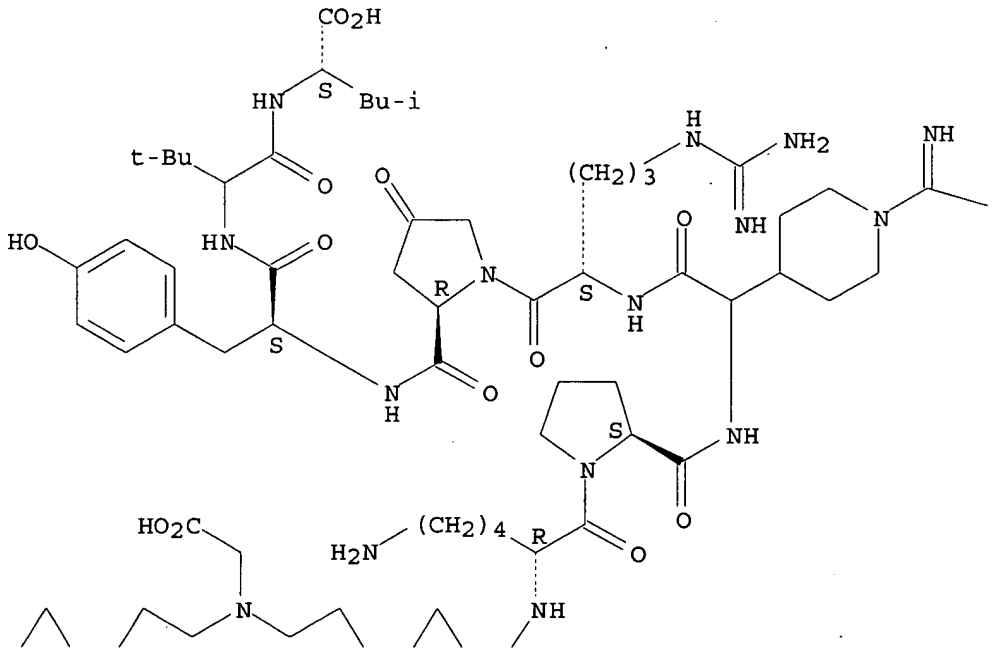

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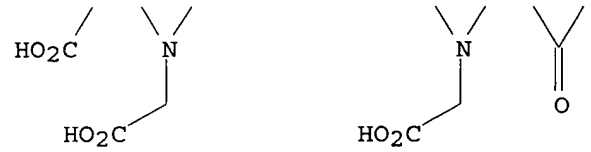
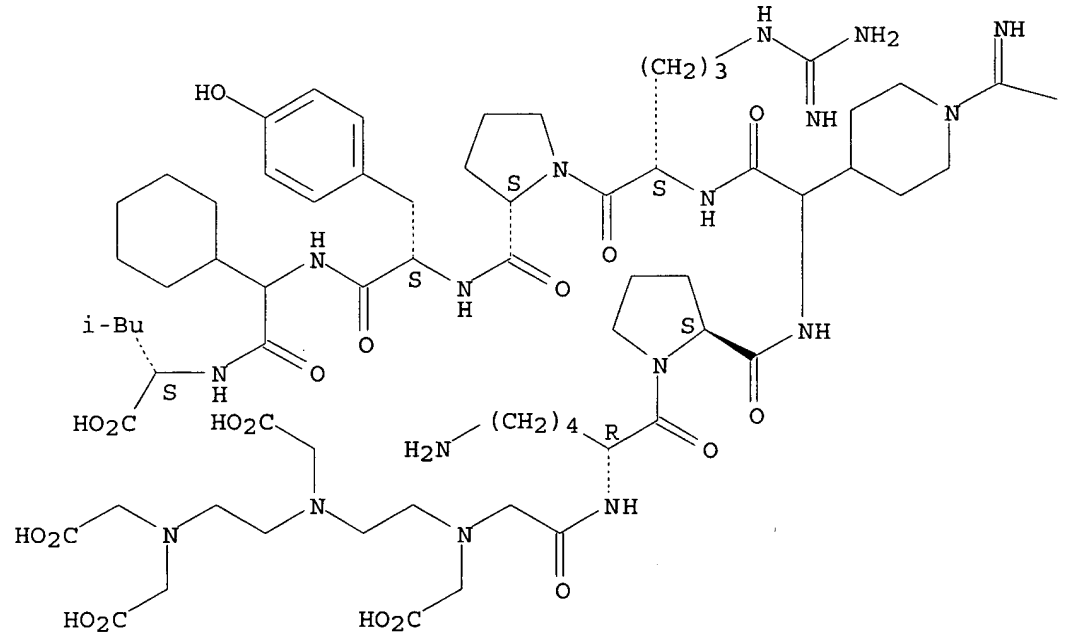


RN 314270-46-7 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-2-cyclohexylglycyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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RN 314270-47-8 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-D-tyrosyl-3-methylvalyl- (9CI) (CA

INDEX NAME)

Absolute stereochemistry.

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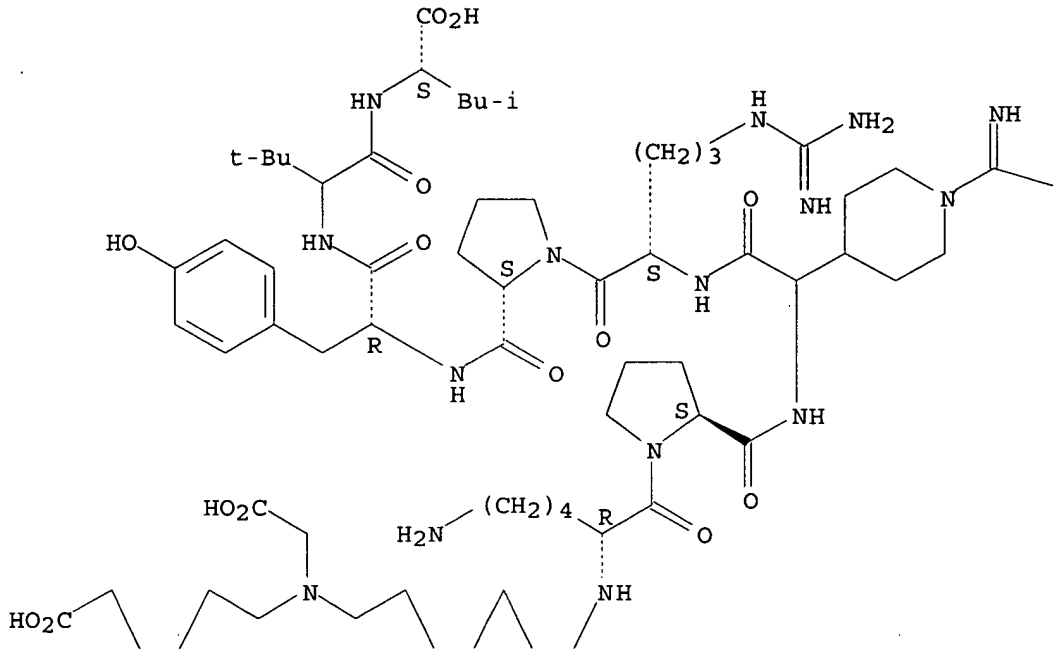

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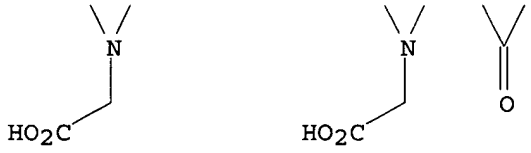

RN 314270-48-9 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-3-[1-(aminoiminomethyl)-4-piperidinyl]alanyl-L-arginyl-L-prolyl-L-tyrosyl-3-methylvalyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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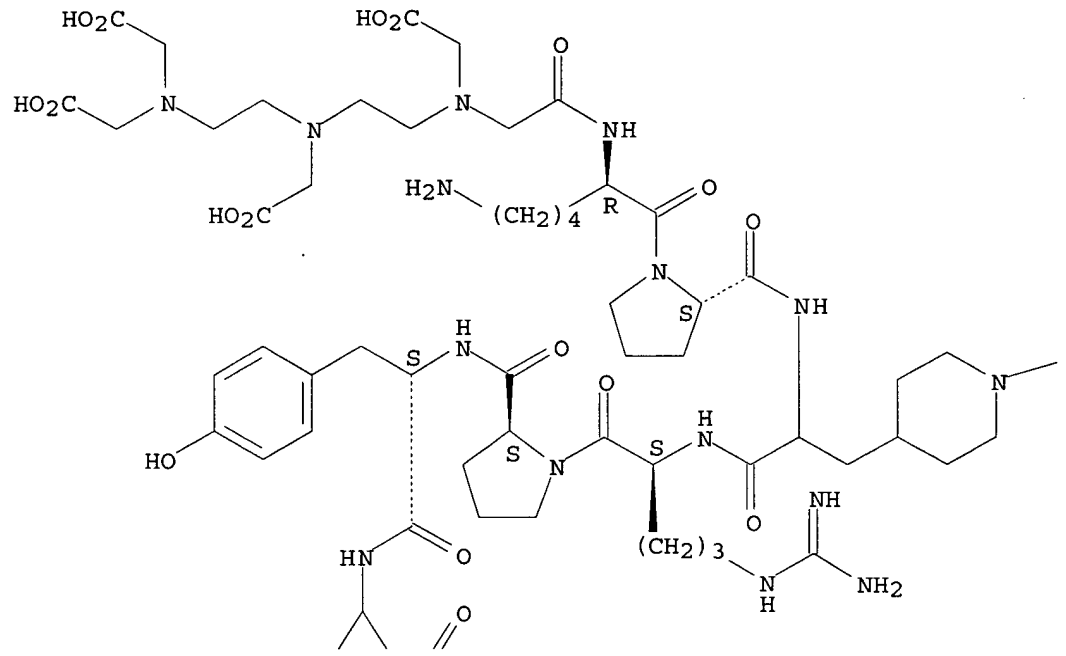

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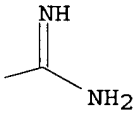

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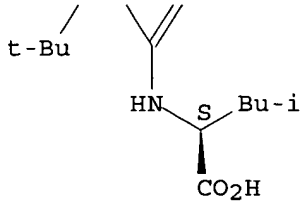
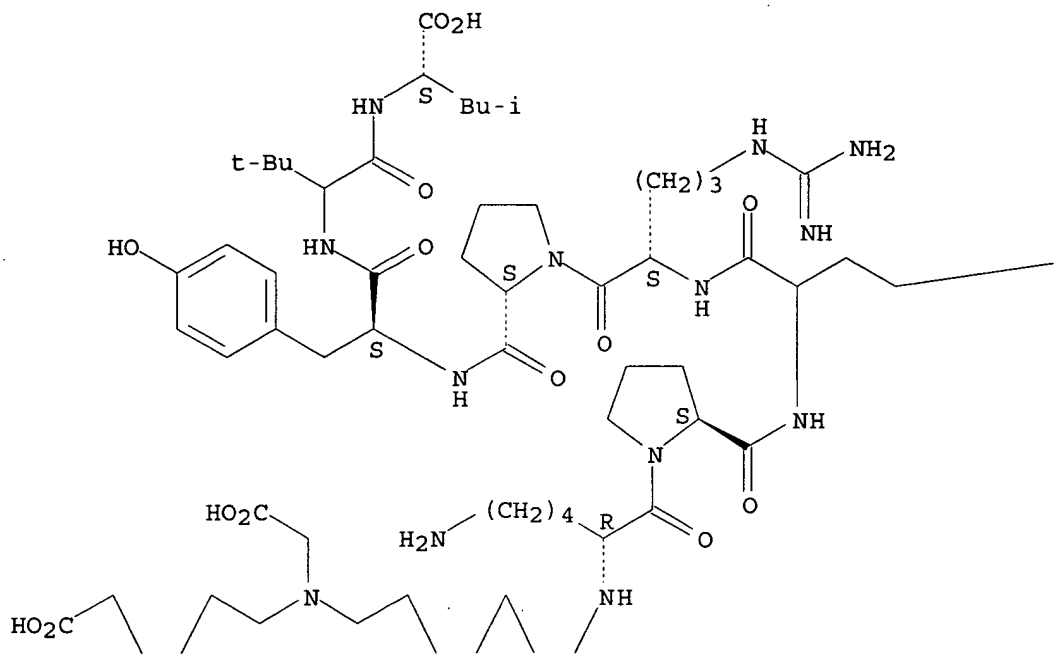


Searched by Barb O'Bryen, STIC 2-2518

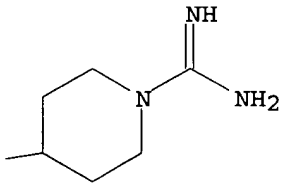
RN 314270-49-0 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-α-amino-1-(aminoiminomethyl)-4-piperidinebutanoyl-L-arginyl-L-prolyl-L-tyrosyl-3-methylvalyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

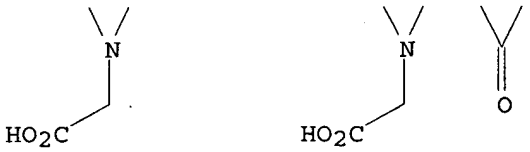
PAGE 1-A



PAGE 1-B



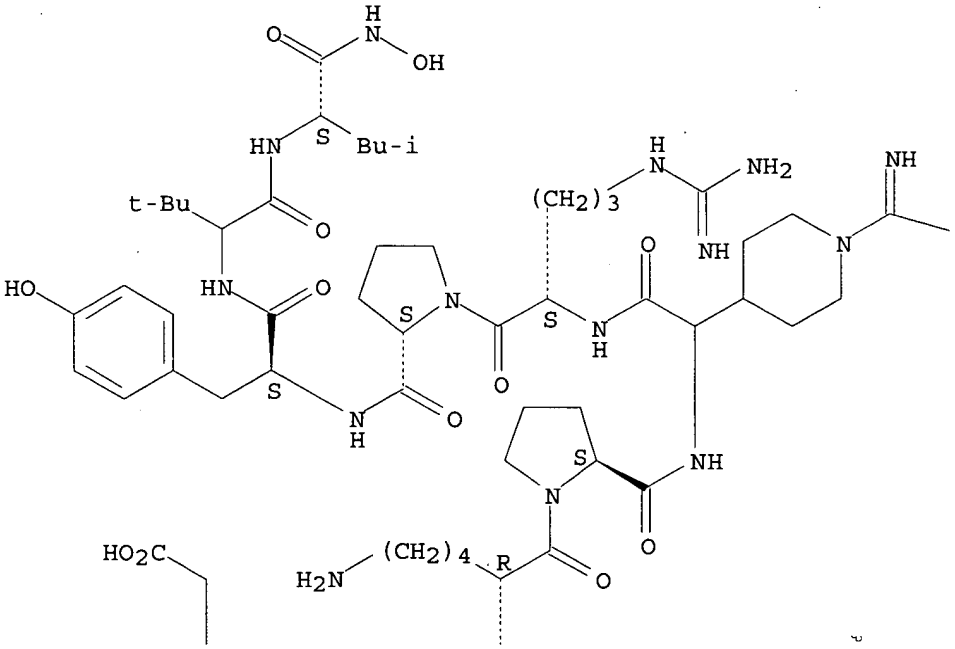
PAGE 2-A



RN 314270-50-3 CAPLUS
CN L-Leucinamide, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methylvalyl-N-hydroxy-(9CI) (CA INDEX NAME)

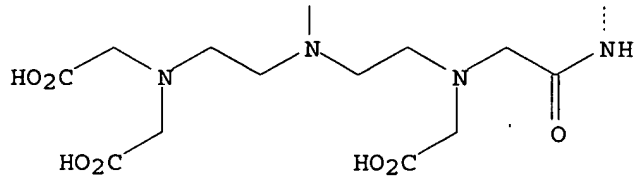
Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

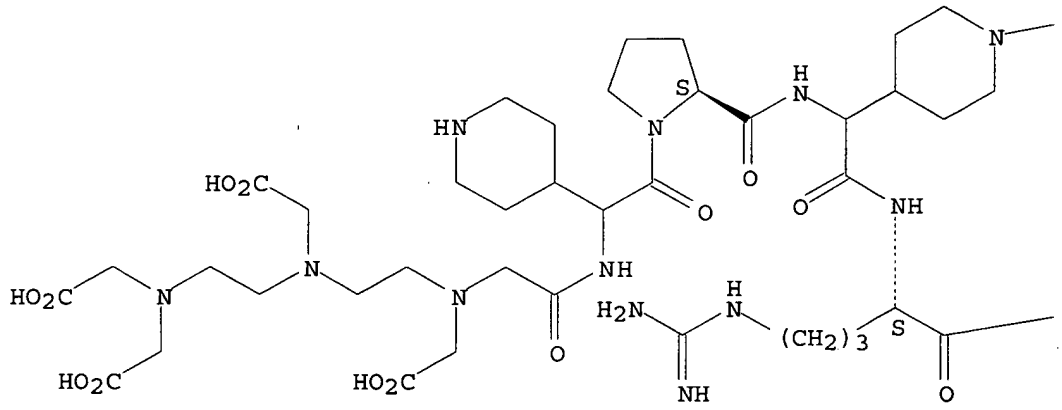
PAGE 2-A



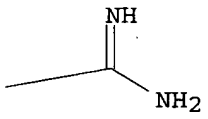
RN 314295-66-4 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-2-(4-piperidinyl)glycyl-L-prolyl-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methylvalyl- (9CI) (CA INDEX NAME)

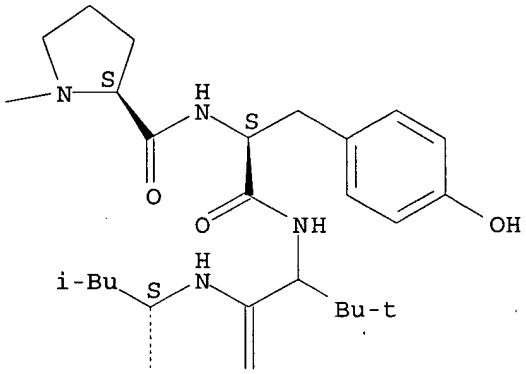
Absolute stereochemistry.

PAGE 1-A

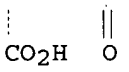


PAGE 1-B





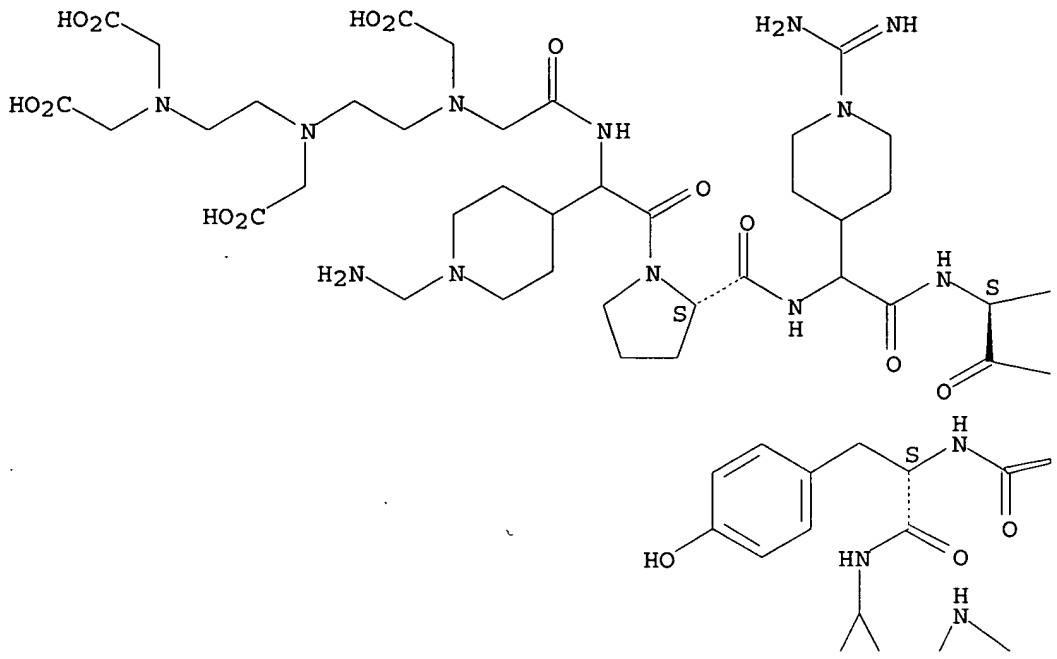
PAGE 2-B



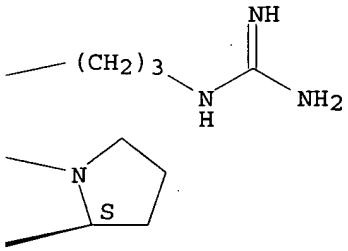
RN 314295-67-5 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-2-[1-(aminomethyl)-4-piperidinyl]glycyl-L-prolyl-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methylvalyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

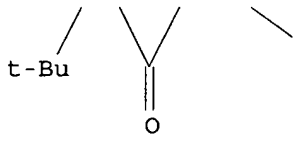


PAGE 1-B

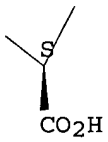


Bu-i

PAGE 2-A



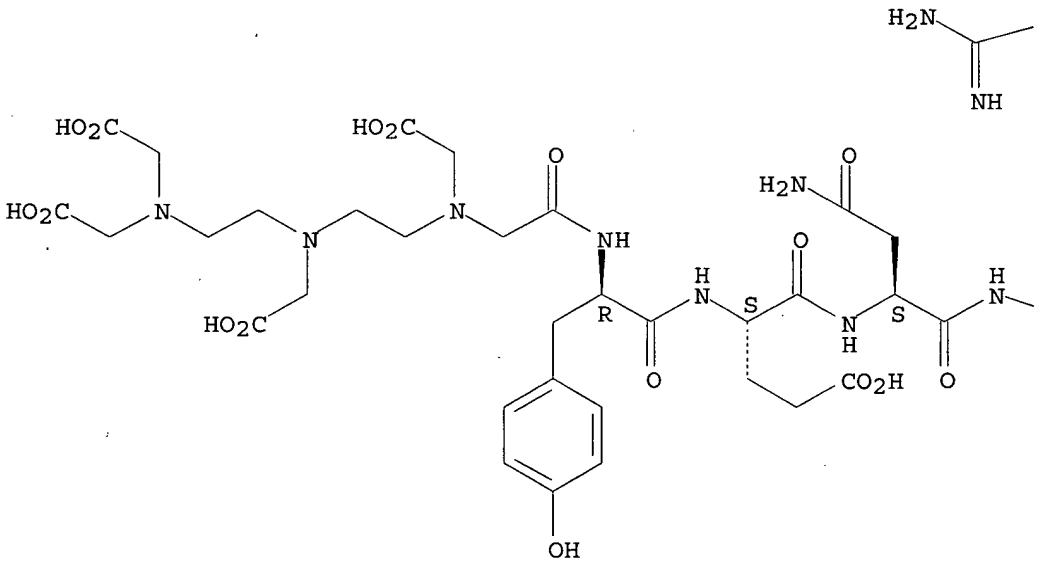
PAGE 2-B



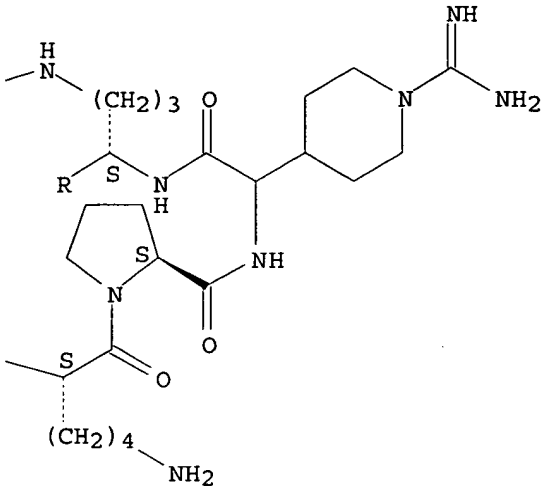
RN 314295-68-6 CAPLUS
CN Alanine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-tyrosyl-L-α-glutamyl-L-asparaginyl-L-lysyl-L-prolyl-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methylvalyl-3-cyclohexyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

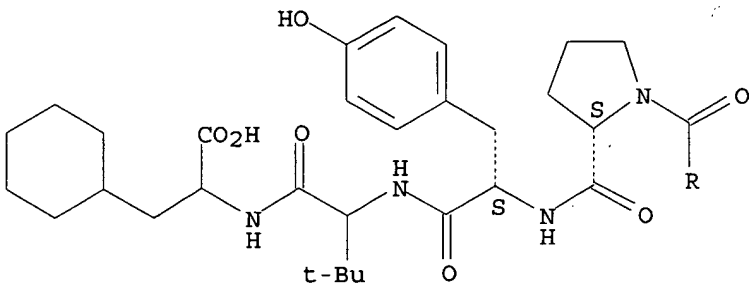
PAGE 1-A



PAGE 1-B



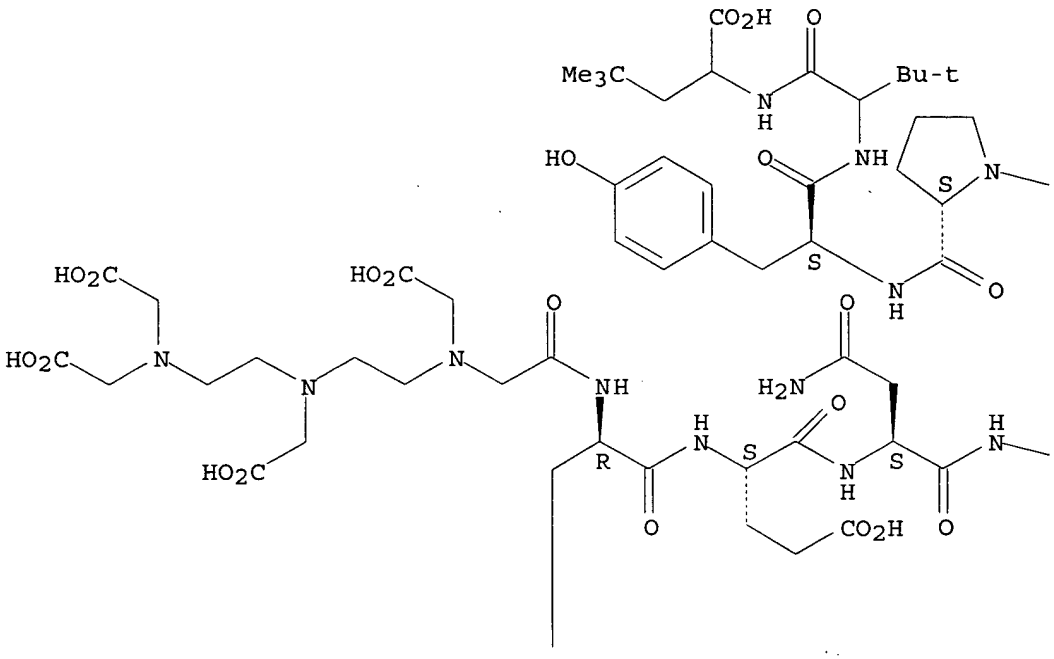
PAGE 2-A



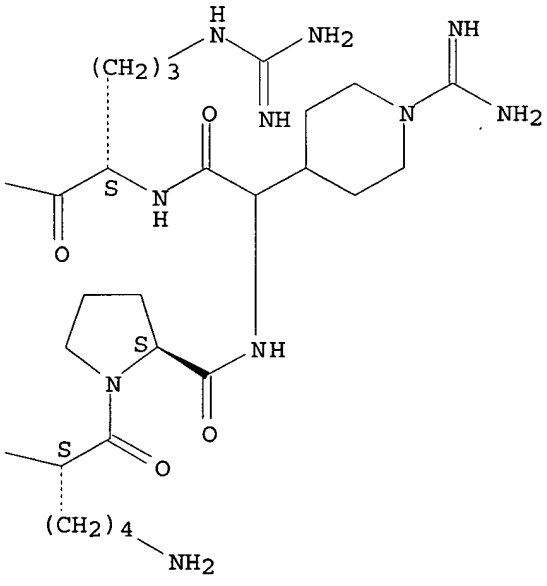
RN 314295-69-7 CAPLUS
CN Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-tyrosyl-L-α-glutamyl-L-asparaginyl-L-lysyl-L-prolyl-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methylvalyl-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

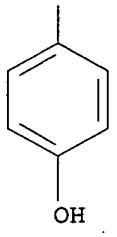
PAGE 1-A



PAGE 1-B



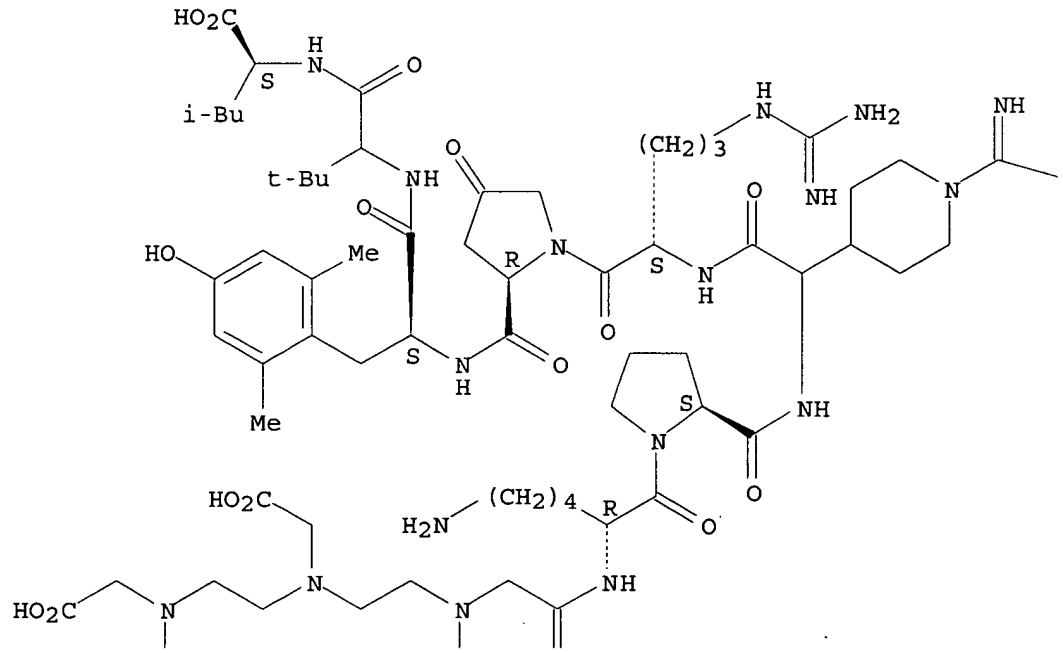
PAGE 2-A



RN 314295-70-0 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-4-oxo-D-prolyl-2,6-dimethyl-L-tyrosyl-3-methylvalyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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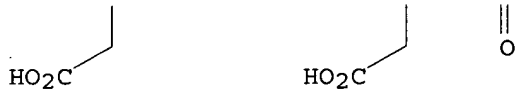
PAGE 2-A



RN 314295-71-1 CAPLUS
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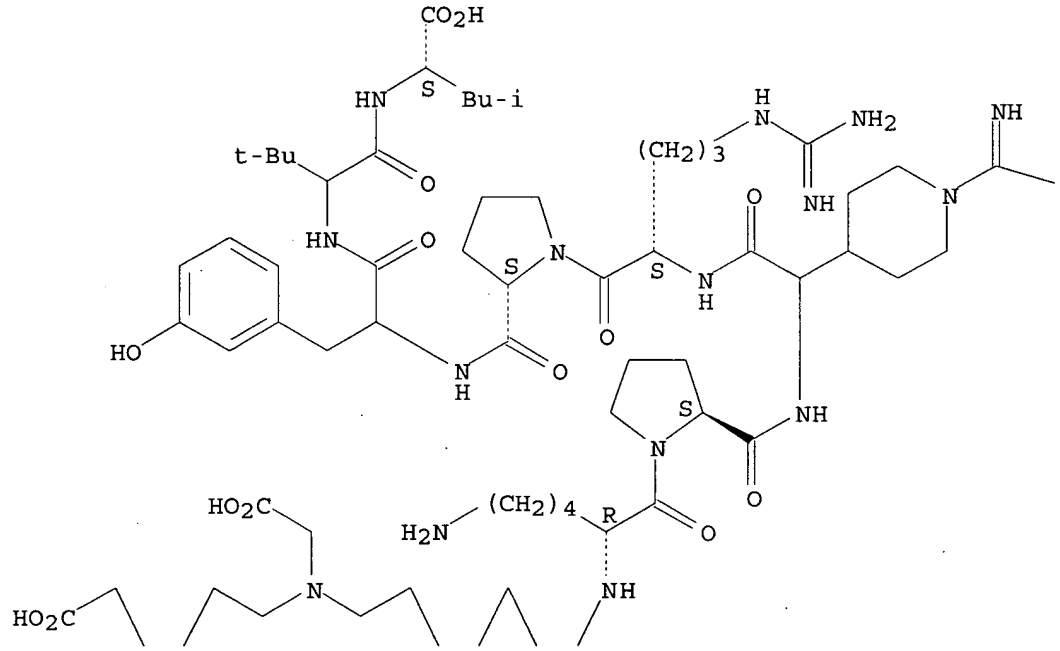
Absolute stereochemistry.

PAGE 1-A



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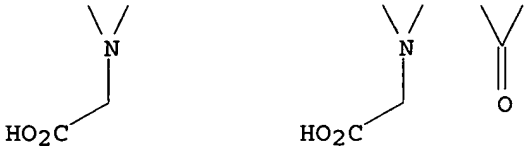
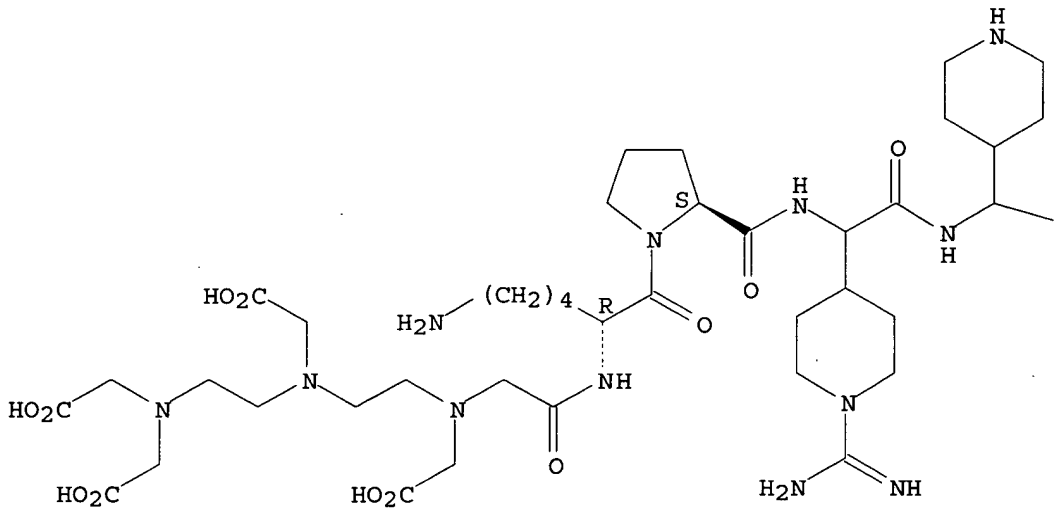
PAGE 2-A



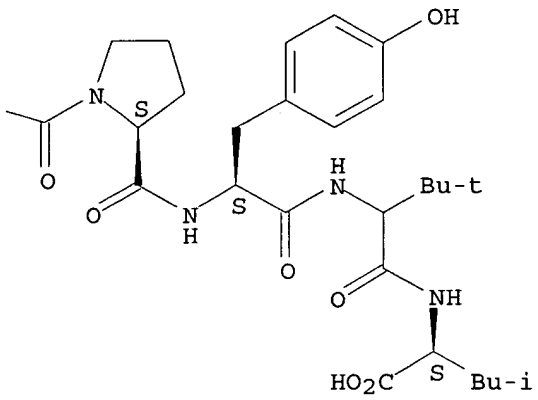
RN 314295-72-2 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-2-(4-piperidinyl)glycyl-L-prolyl-L-tyrosyl-3-methylvalyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



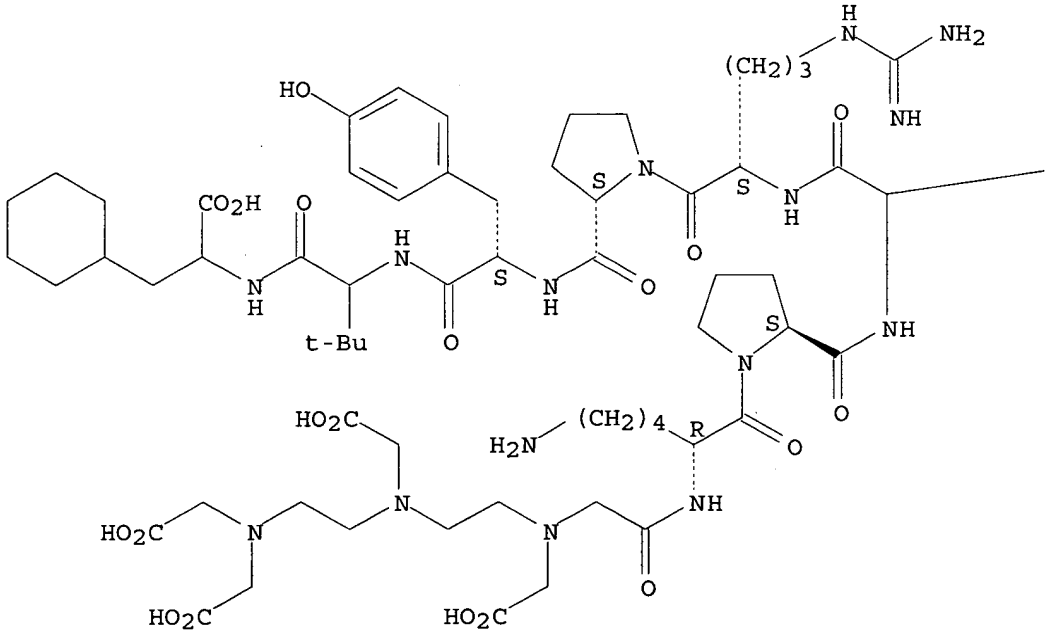
PAGE 1-B



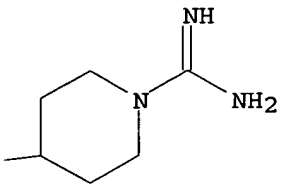
RN 314295-74-4 CAPLUS
CN Alanine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methylvalyl-3-cyclohexyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



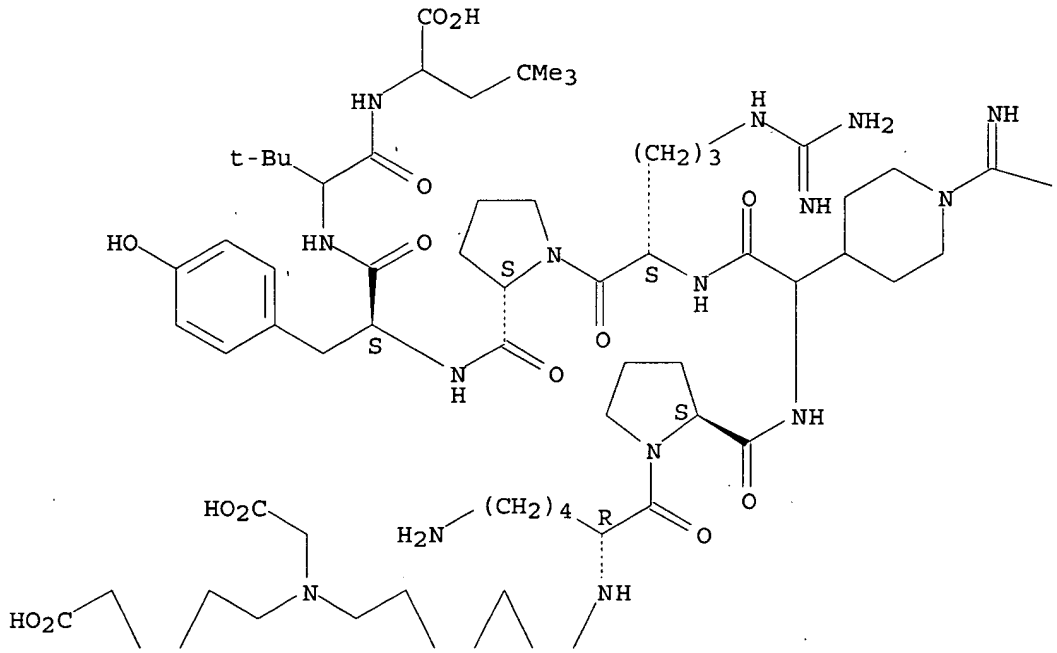
PAGE 1-B



RN 314295-75-5 CAPLUS
CN Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-D-lysyl-L-prolyl-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methylvalyl-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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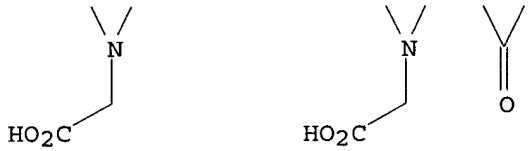
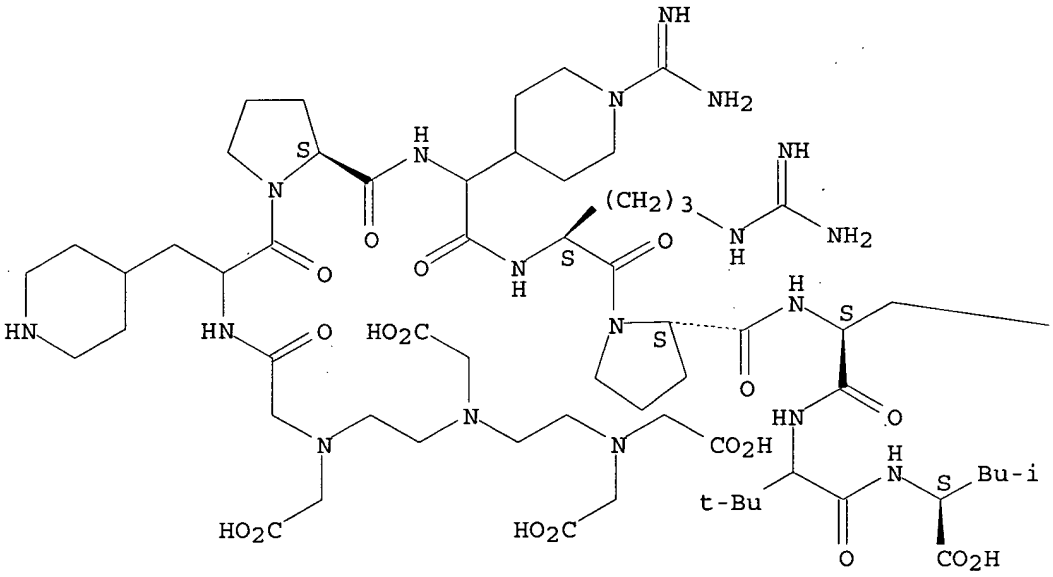
PAGE 2-A



RN 314295-76-6 CAPLUS
CN L-Leucine, N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]-N-(carboxymethyl)glycyl-3-(4-piperidinyl)alanyl-L-prolyl-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methylvalyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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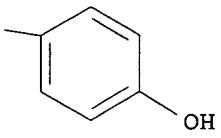


L45 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:575856 CAPLUS
DOCUMENT NUMBER: 141:12065
TITLE: Stabilised 111In-labelled DTPA- and DOTA-conjugated neurotensin analogues for imaging and therapy of exocrine pancreatic cancer
AUTHOR(S): de Visser, M.; Janssen, P. J. J. M.; Srinivasan, A.; Reubi, J. C.; Waser, B.; Erion, J. L.; Schmidt, M. A.; Krenning, E. P.; de Jong, M.
CORPORATE SOURCE: Department of Nuclear Medicine, Erasmus MC, Rotterdam, 3015 GD, Neth.
SOURCE: European Journal of Nuclear Medicine and Molecular Imaging (2003), 30(8), 1134-1139
CODEN: EJNMA6; ISSN: 1619-7070
PUBLISHER: Springer-Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 28 Jul 2003
AB Neurotensin (NT) receptors are overexpressed in exocrine pancreatic cancer and Ewing's sarcoma. The potential utility of native NT in cancer diagnosis and therapy is, however, limited by its rapid degradation in vivo. Therefore, NT analogs were synthesized with modified lysine and arginine derivs. to enhance stability and coupled either to DTPA, to enable high specific activity labeling with indium-111 for imaging, or to DOTA, to enable high specific activity labeling with β-emitting radionuclides, such as lutetium-177 and yttrium-90. Based on serum stability (4 h incubation at 37°C in human serum) and receptor binding affinity, the five most promising analogs were selected and further evaluated in in vitro internalization studies in human colorectal adenocarcinoma HT29 cells, which overexpress NT receptors. All five NT analogs bound with high affinity to NT receptors on human exocrine pancreatic tumor sections. The analogs could be labeled with 111In to a high specific activity. The 111In-labeled compds. were found to be very stable in serum. Incubation of HT29 cells with the 111In-labeled analogs at 37°C showed rapid receptor-mediated uptake and internalization. The most promising analog, peptide 2530 [DTPA-(Pip)Gly-Pro-(PipAm)Gly-Arg-Pro-Tyr-tBuGly-Leu-OH] was further tested in vivo in a biodistribution study using HT29 tumor-bearing nude mice. The results of this study showed low percentages of injected dose per g tissue of this 111In-labeled 2530 analog in receptor-neg.

organs like blood, spleen, pancreas, liver, muscle and femur. Good uptake was found in the receptor-pos. HT29 tumor and high uptake was present in the kidneys. Co-injection of excess unlabeled NT significantly reduced tumor uptake, showing that tumor uptake is a receptor-mediated process. With their enhanced stability, maintained high receptor affinity and rapid receptor-mediated internalization, the 111In-labeled DTPA- and DOTA-conjugated NT analogs are excellent candidates for imaging and therapy of exocrine pancreatic cancer, peptide 2530 being the most promising analog.

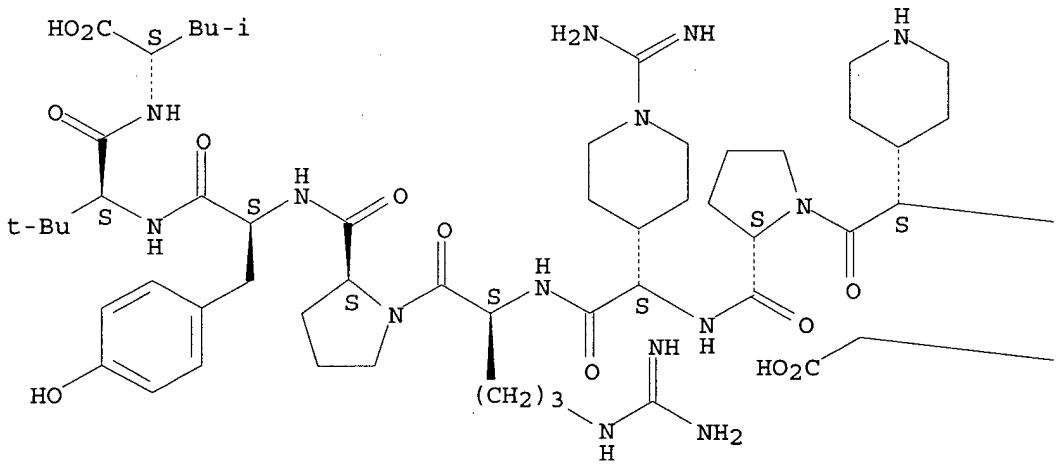
IT **694452-76-1DP**, In(111)-labeled **697236-75-2P**
697236-79-6P 697236-89-8P 697236-90-1P
RL: DGN (Diagnostic use); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(stabilized 111In-labeled DTPA- and DOTA-conjugated neurotensin analogs for imaging and therapy of exocrine pancreatic cancer)

RN 694452-76-1 CAPLUS

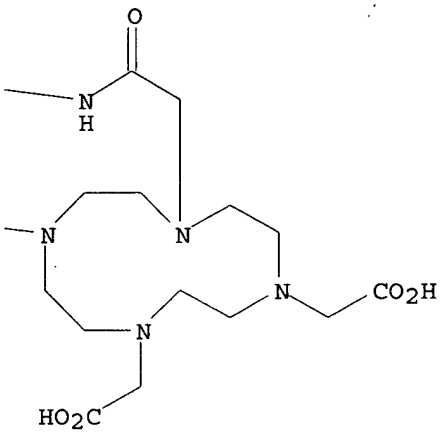
CN L-Leucine, (2S)-2-(4-piperidinyl)-N-[[4,7,10-tris(carboxymethyl)-1,4,7,10-tetraazacyclododec-1-yl]acetyl]glycyl-L-prolyl-(2S)-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methyl-L-valyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



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CN Indate(2-)-111In, [N-[(carboxy-κO)methyl]-N-[2-[[(carboxy-κO)methyl][2-[[(carboxy-κO)methyl](carboxymethyl)amino-κN]ethyl]amino-κN]ethyl]glycyl-κN-(2S)-2-(4-piperidinyl)glycyl-L-prolyl-(2S)-2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methyl-L-valyl-L-leucinato(5-)]-, dihydrogen (9CI) (CA INDEX NAME)

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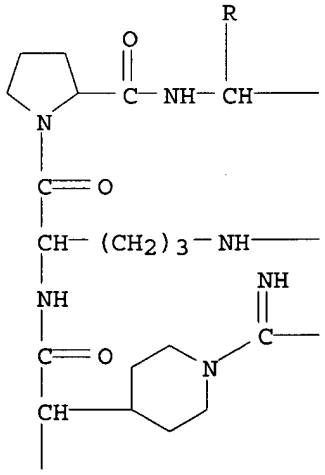
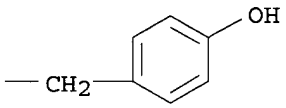
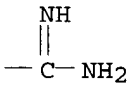
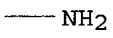


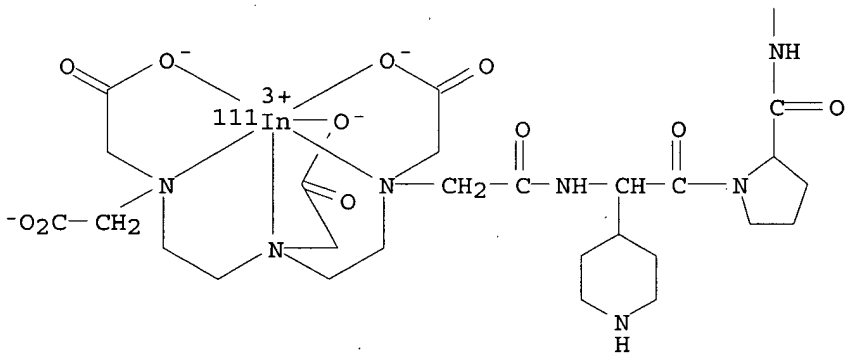
PAGE 1-B

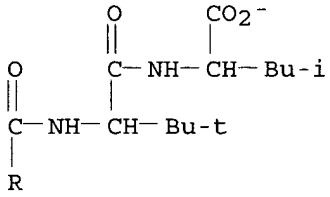






PAGE 2-A





PAGE 2-B

●2 H^+

RN 697236-79-6 CAPLUS
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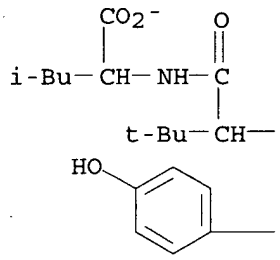
PAGE 1-A



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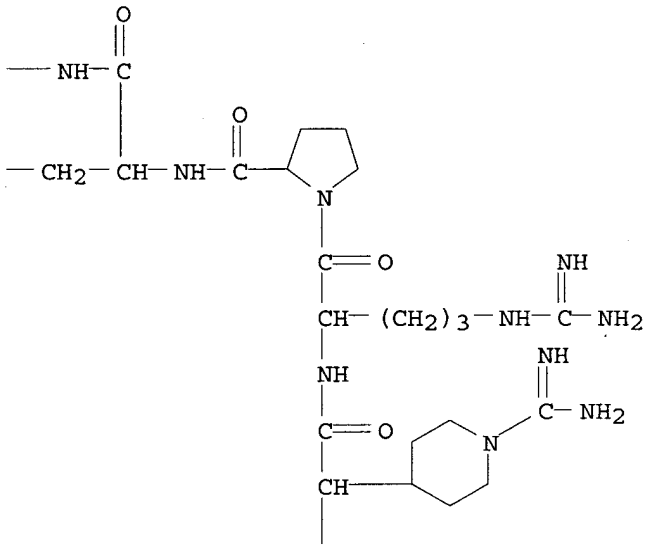

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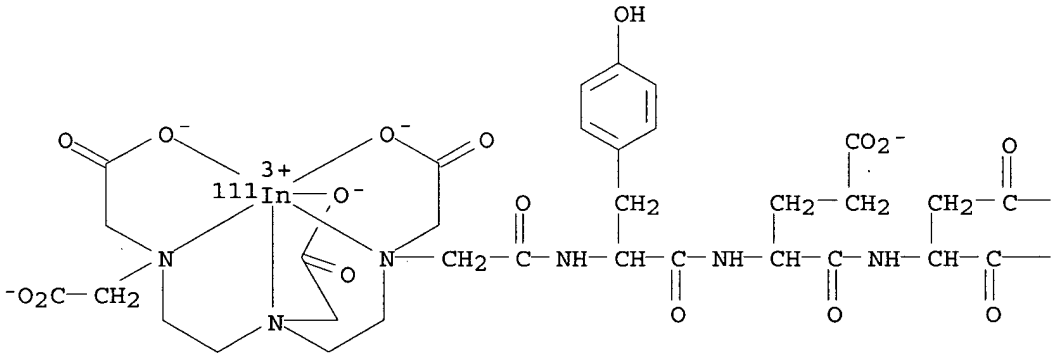
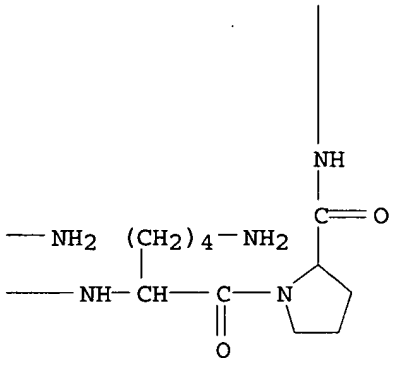


●3 H^+

PAGE 2-B



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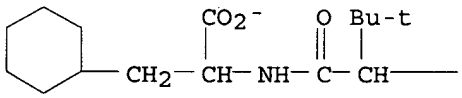
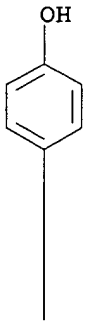
PAGE 1-A





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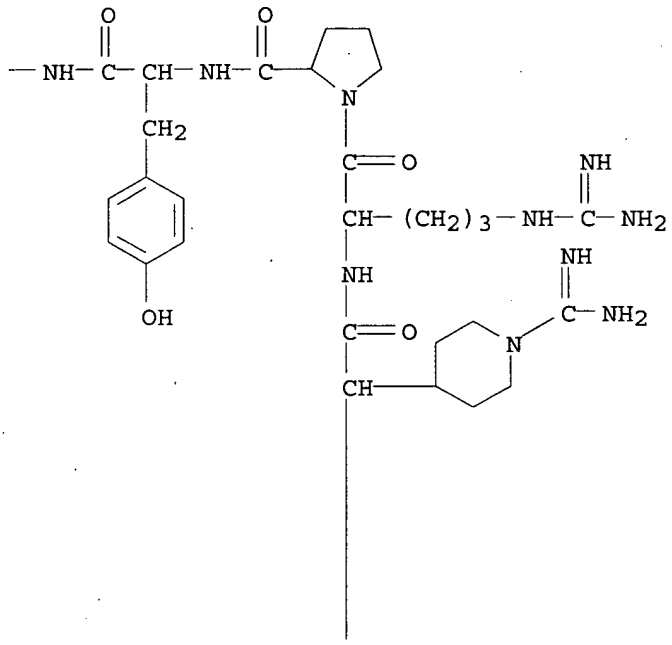

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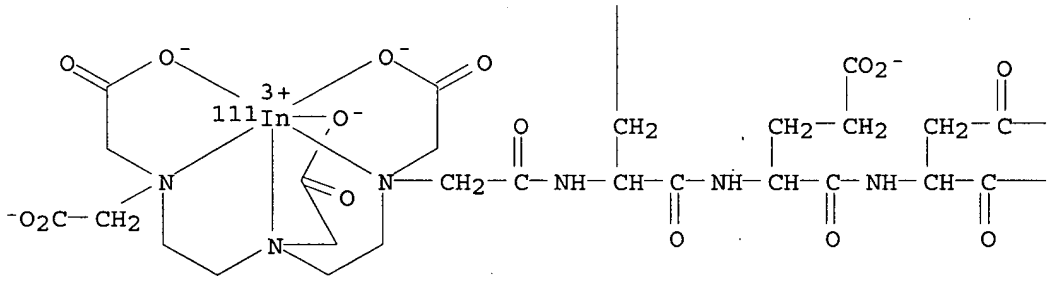
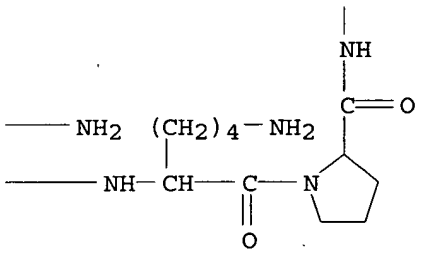


● 3 H^+

PAGE 2-B



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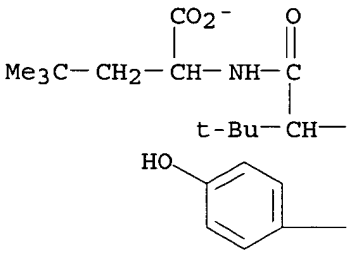
PAGE 1-A



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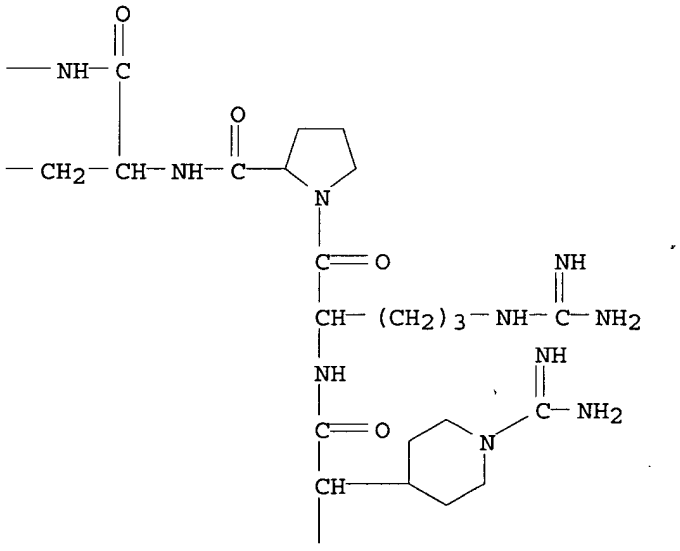

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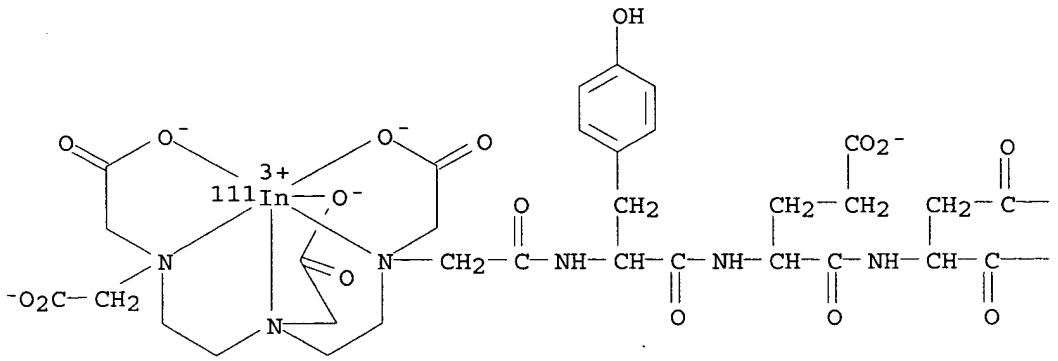
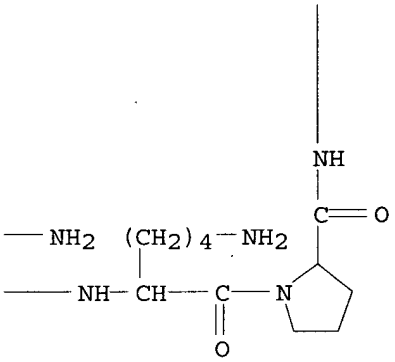


●3 H^+

PAGE 2-B



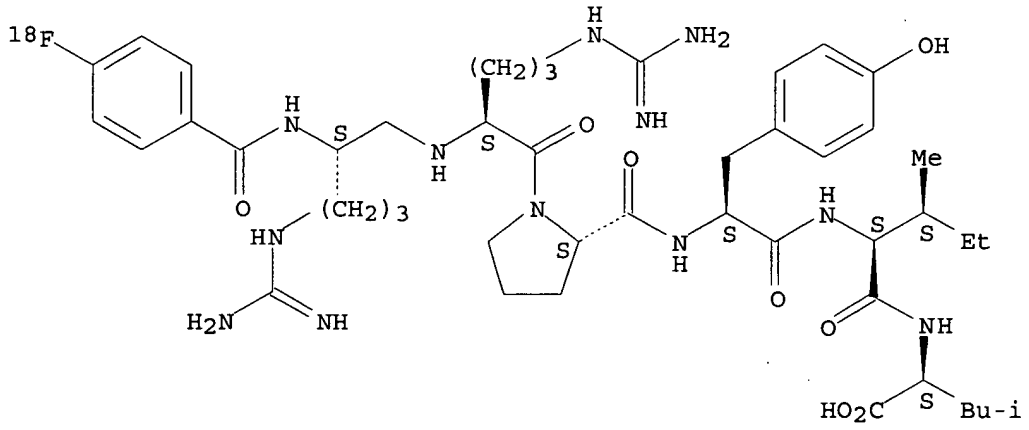
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L45 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:692681 CAPLUS
DOCUMENT NUMBER: 138:250779
TITLE: Synthesis of potent and enzymatically stable 4-18F-benzoyl-NT(8-13) analogs for tumor diagnosis using PET
AUTHOR(S): Iterbeke, K.; Bergmann, R.; Johanssen, B.; Torok, G.; Laus, G.; Tourwe, D.
CORPORATE SOURCE: Department of Organic Chemistry, Vrije Universiteit Brussel, Brussels, B-1050, Belg.
SOURCE: Peptides: The Wave of the Future, Proceedings of the Second International and the Seventeenth American Peptide Symposium, San Diego, CA, United States, June 9-14, 2001 (2001), 984-985. Editor(s): Lebl, Michal; Houghten, Richard A. American Peptide Society: San Diego, Calif.
CODEN: 69DBAL; ISBN: 0-9715560-0-8

Searched by Barb O'Bryen, STIC 2-2518

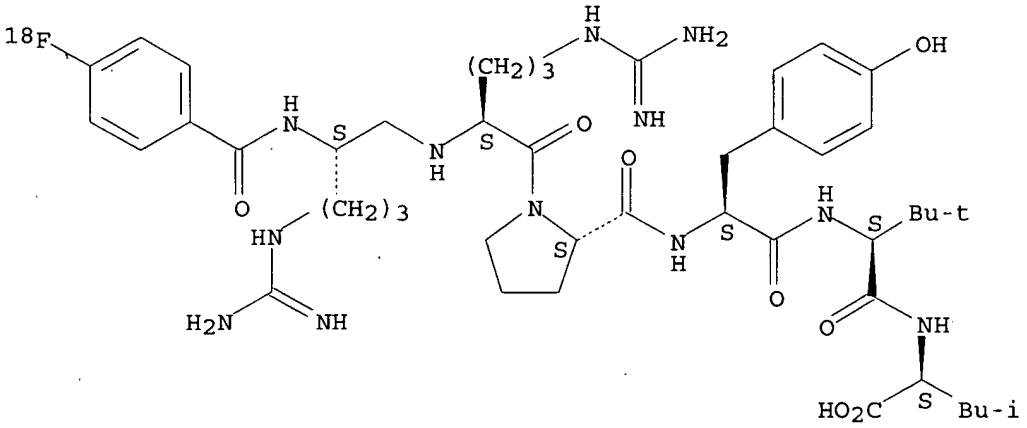
DOCUMENT TYPE: Conference
LANGUAGE: English
ED Entered STN: 13 Sep 2002
AB The analogs of the biol. part of neurotensin (NT), NT(8-13), which were developed as potential PET-tracers were prepared by solid phase peptide synthesis on a Merrifield resin using Boc main-chain protected amino acids. Radiolabeling was performed using 0.7 mg of the resp. peptide in a N-succinimidyl-4-[18F]fluorobenzoate solution on 25% CH3CN in Koltthoff's buffer at 45° for 50 min. IC50 values for the non-radioactive compds. showed that NT-1 and NT-2 have comparable IC50 values as the native NT while NT-3 and NT-4 displayed a loss in binding affinity. Arterial blood samples showed very fast degradation of 4-18F-benzoyl-NT-1 and 4-18F-benzoyl-NT-2. 4-18F-benzoyl-NT-4, and to a lesser extent 4-18F-benzoyl-NT-3, showed an increased in vivo stability. Ex vivo autoradiog. on HT-29 tumor bearing mice displayed an increased tumor uptake for 4-18F-benzoyl-NT-4 making it potential candidate for use in diagnosis of NT receptor-containing carcinomas with PET.
IT **266352-47-0P 406486-48-4P 502923-55-9P 502923-56-0P**
RL: DGN (Diagnostic use); PKT (Pharmacokinetics); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(potent and metabolically stable 4-18F-benzoyl-neurotensin(8-13) analogs preparation for PET tumor imaging)
RN 266352-47-0 CAPLUS
CN L-Leucine, N2-[(2S)-5-[(aminoiminomethyl)amino]-2-[[4-(fluoro-18F)benzoyl]amino]pentyl]-L-arginyl-L-prolyl-L-tyrosyl-L-isoleucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



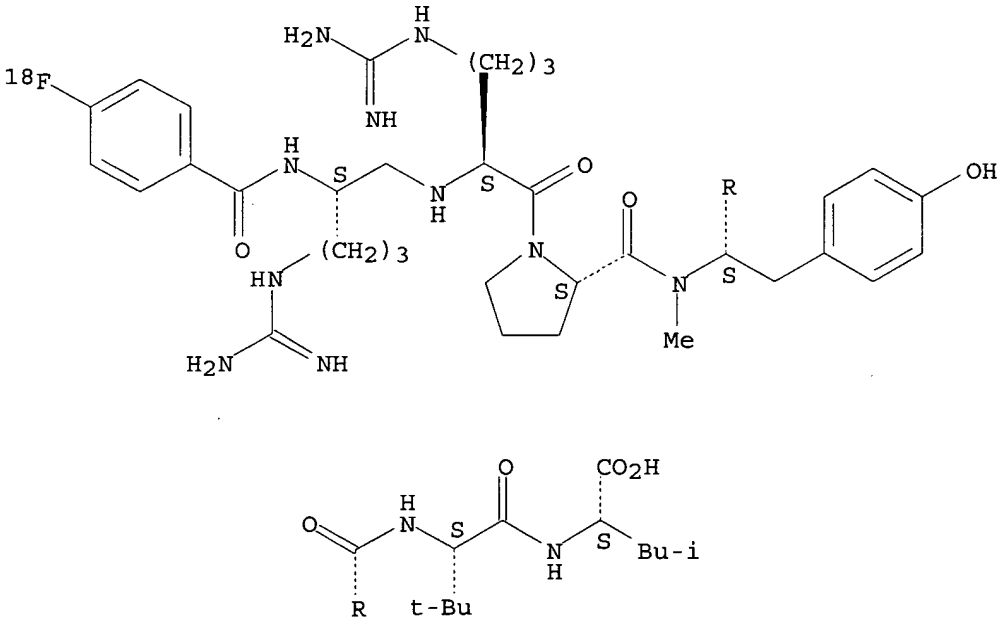
RN 406486-48-4 CAPLUS
CN L-Leucine, N2-[(2S)-5-[(aminoiminomethyl)amino]-2-[[4-(fluoro-18F)benzoyl]amino]pentyl]-L-arginyl-L-prolyl-L-tyrosyl-3-methyl-L-valyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



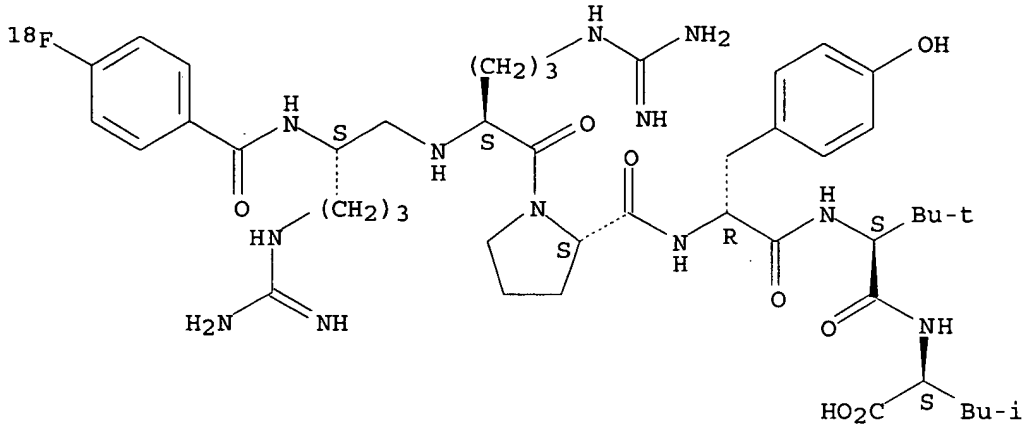
RN 502923-55-9 CAPLUS
CN L-Leucine, N2-[(2S)-5-[(aminoiminomethyl)amino]-2-[[4-(fluoro-18F)benzoyl]amino]pentyl]-L-arginyl-L-prolyl-N-methyl-L-tyrosyl-3-methyl-L-valyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 502923-56-0 CAPLUS
CN L-Leucine, N2-[(2S)-5-[(aminoiminomethyl)amino]-2-[[4-(fluoro-18F)benzoyl]amino]pentyl]-L-arginyl-L-prolyl-D-tyrosyl-3-methyl-L-valyl- (9CI) (CA INDEX NAME)

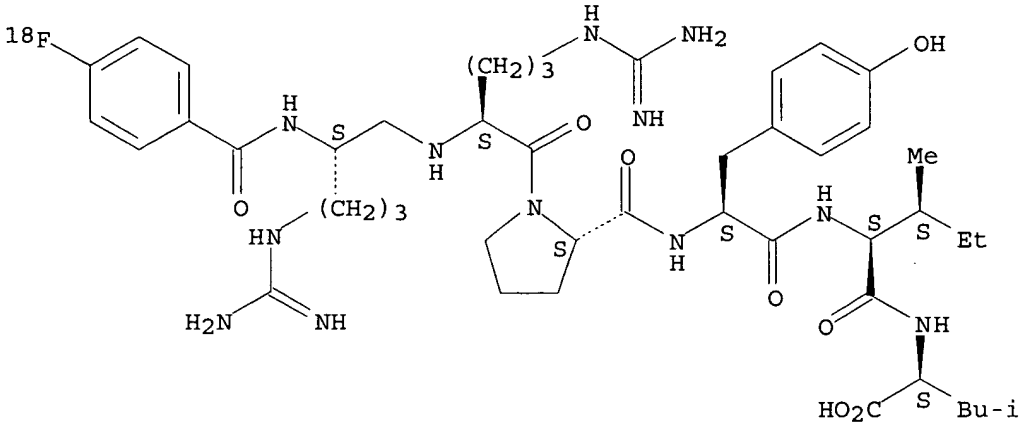
Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

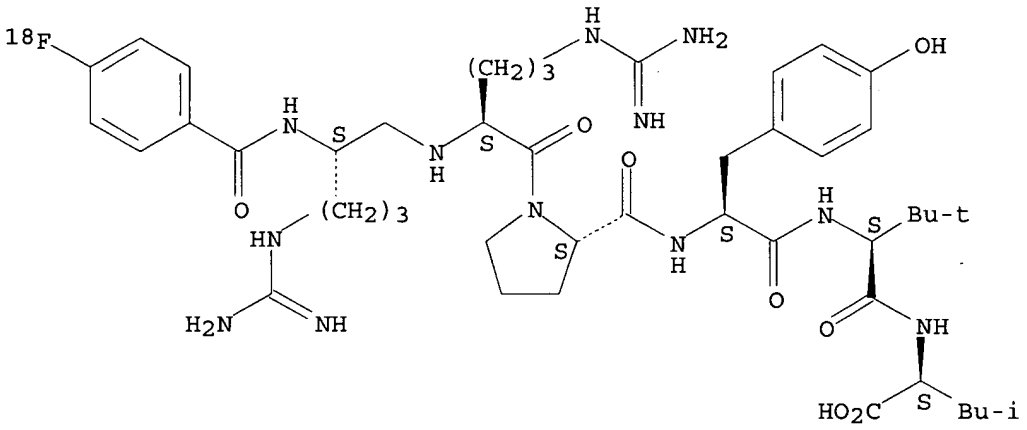
L45 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:174815 CAPLUS
DOCUMENT NUMBER: 137:353283
TITLE: F-18 peptide labelling: neurotensin derivatives
AUTHOR(S): Scheunemann, M.; Mading, P.; Bergmann, R.; Steinbach, J.; Iterbeke, K.; Tourwe, D.; Johannsen, B.
CORPORATE SOURCE: Institut fur Bioanorganische und Radiopharmazeutische Chemie, Dresden, 01314, Germany
SOURCE: Synthesis and Applications of Isotopically Labelled Compounds, Proceedings of the International Symposium, 7th, Dresden, Germany, June 18-22, 2000 (2001), Meeting Date 2000, 380-383. Editor(s): Pleiss, Ulrich; Voges, Rolf. John Wiley & Sons Ltd.: Chichester, UK.
CODEN: 69CIJC; ISBN: 0-471-49501-8
DOCUMENT TYPE: Conference
LANGUAGE: English
ED Entered STN: 11 Mar 2002
AB A symposium report. N-succinimidyl 4-[18F]fluorobenzoate was applied to the specific radiolabeling of non-lysine containing oligopeptides of neurotensin (NT) such as hexapeptide NT(8-13), [Arg8Ψ(CH2NH)Arg9]NT(8-13), and [Arg8Ψ(CH2NH)Arg9,Tle12]NT(8-13) at the α-amino group of the N-terminal arginine unit.
IT **266352-47-0P 406486-48-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(fluorine-18 labeling of neurotensin derivs.)
RN 266352-47-0 CAPLUS
CN L-Leucine, N2-[(2S)-5-[(aminoiminomethyl)amino]-2-[[4-(fluoro-18F)benzoyl]amino]pentyl]-L-arginyl-L-prolyl-L-tyrosyl-L-isoleucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 406486-48-4 CAPLUS
CN L-Leucine, N2-[(2S)-5-[(aminoiminomethyl)amino]-2-[[4-(fluoro-18F)benzoyl]amino]pentyl]-L-arginyl-L-prolyl-L-tyrosyl-3-methyl-L-valyl-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



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L45 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:894782 CAPLUS
DOCUMENT NUMBER: 134:202782
TITLE: Increased serum stability of neurotensin analogs containing arginine mimics
AUTHOR(S): Schmidt, Michelle A.; Erion, Jack L.; Chinen, Lori K.; Bugaj, Joseph E.; Wilhelm, R. Randy; Srinivasan, Ananth
CORPORATE SOURCE: Discovery Research, Mallinckrodt, Inc., Hazelwood, MO, 63042, USA
SOURCE: Peptides for the New Millennium, Proceedings of the American Peptide Symposium, 16th, Minneapolis, MN, United States, June 26-July 1, 1999 (2000), Meeting Date 1999, 634-635. Editor(s): Fields, Gregg B.; Tam, James P.; Barany, George. Kluwer Academic Publishers:

Dordrecht, Neth.
CODEN: 69ATHX
DOCUMENT TYPE: Conference
LANGUAGE: English
ED Entered STN: 21 Dec 2000

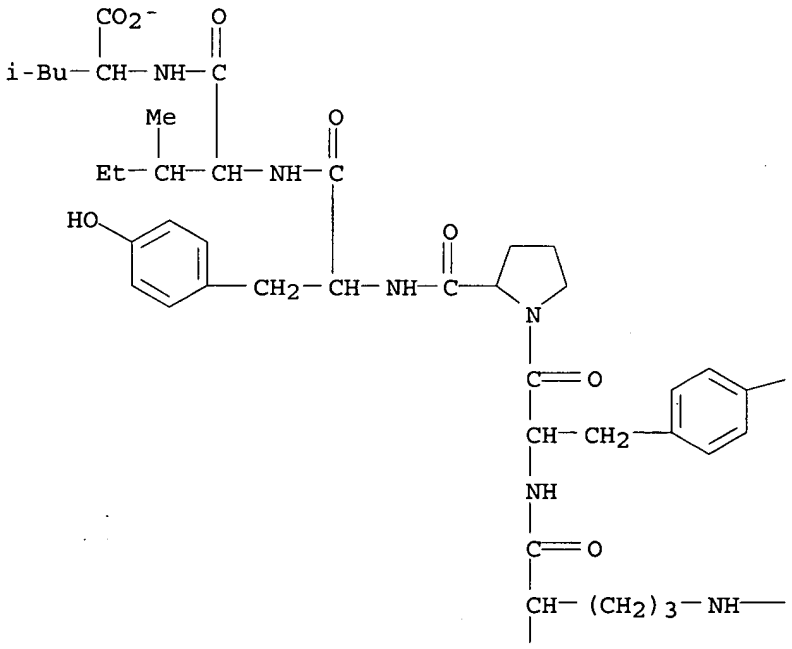
AB Novel neurotensin derivs. were prepared by initially replacing one or both arginines of NT(6-13) with a com.-available arginine mimic. While serum stability was improved by the incorporation of Arg mimics, there was still less than 20% intact peptide remaining at 4 h in each case. The presence of serum degradation products with slightly shorter retention times than the intact peptide in HPLC anal. suggested that another region of instability was near the C-terminus (data not shown). To address this issue, derivs. with C-terminal modifications were prepared which retained the Arg mimics responsible for the highest binding affinity. A dramatic improvement in serum stability was observed with derivs. containing an unnatural amino acid (t-butylGly) or a pseudo-peptide bond; however, only two compds. were still active.

IT **328526-77-8 328526-78-9 328526-79-0**
328526-80-3 328526-81-4 328526-82-5
328526-83-6 328526-85-8
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(increased serum stability of neurotensin analogs containing arginine mimics)

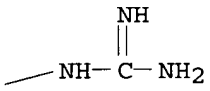
RN 328526-77-8 CAPLUS

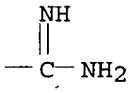
CN Indate(2-)-111In, [N-[(carboxy-κO)methyl]-N-[2-[[(carboxy-κO)methyl][2-[[(carboxy-κO)methyl](carboxymethyl)amino-κN]ethyl]amino-κN]ethyl]glycyl-κN-D-lysyl-L-prolyl-L-arginyl-4-[(aminoiminomethyl)amino]-L-phenylalanyl-L-prolyl-L-tyrosyl-L-isoleucyl-L-leucinato(5-)]-, dihydrogen (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B





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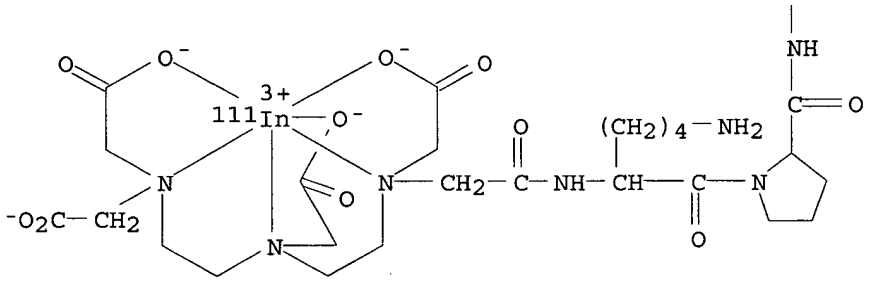
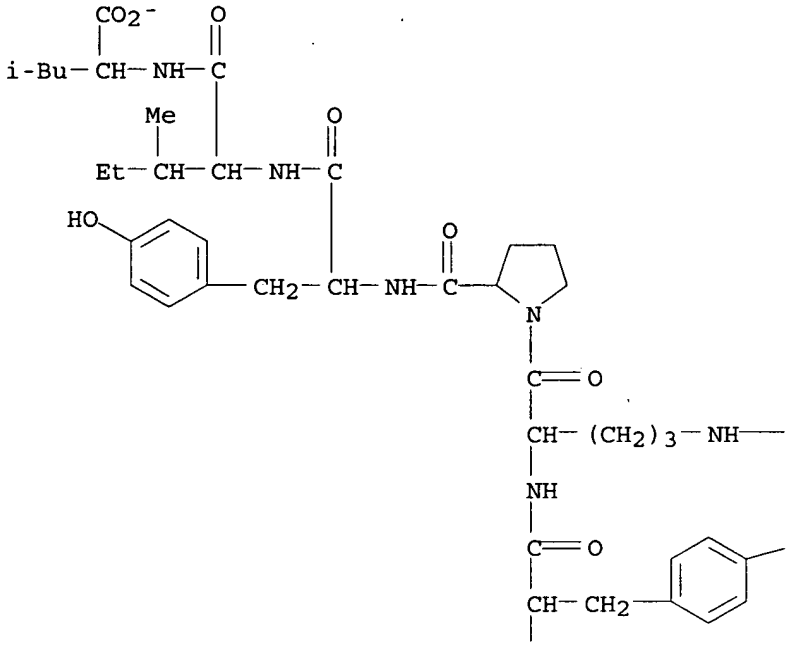


●2 H^+

RN 328526-78-9 CAPLUS

CN Indate(2-)-111In, [N-[(carboxy-κO)methyl]-N-[2-[[(carboxy-κO)methyl][2-[[(carboxy-κO)methyl](carboxymethyl)amino-κN]ethyl]amino-κN]ethyl]glycyl-κN-D-lysyl-L-prolyl-4-[(aminoiminomethyl)amino]-L-phenylalanyl-L-arginyl-L-prolyl-L-tyrosyl-L-isoleucyl-L-leucinato(5-)]-, dihydrogen (9CI) (CA INDEX NAME)

PAGE 1-A



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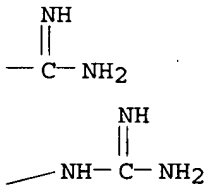

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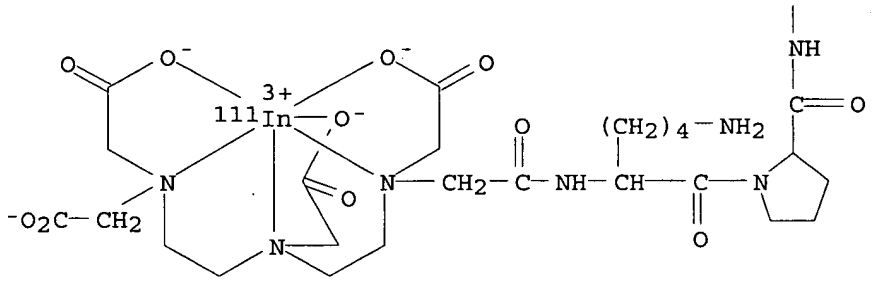
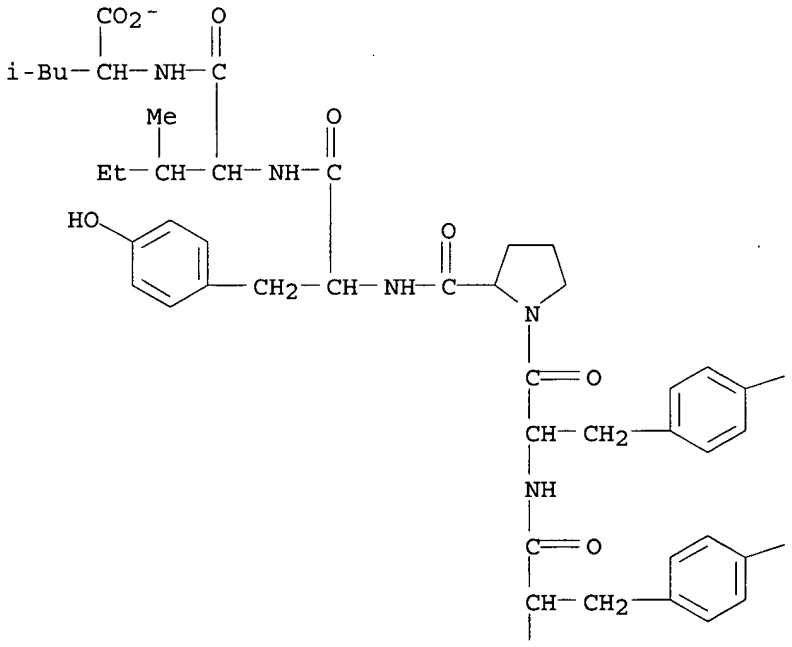


● 2 H^+

RN 328526-79-0 CAPLUS

CN Indate(2-)-111In, [N-[(carboxy-κO)methyl]-N-[2-[[(carboxy-κO)methyl][2-[[(carboxy-κO)methyl](carboxymethyl)amino-κN]ethyl]amino-κN]ethyl]glycyl-κN-D-lysyl-L-prolyl-4-[(aminoiminomethyl)amino]-L-phenylalanyl-4-[(aminoiminomethyl)amino]-L-phenylalanyl-L-prolyl-L-tyrosyl-L-isoleucyl-L-leucinato(5-)]-, dihydrogen (9CI) (CA INDEX NAME)

PAGE 1-A



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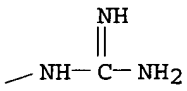

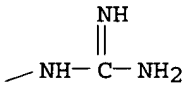

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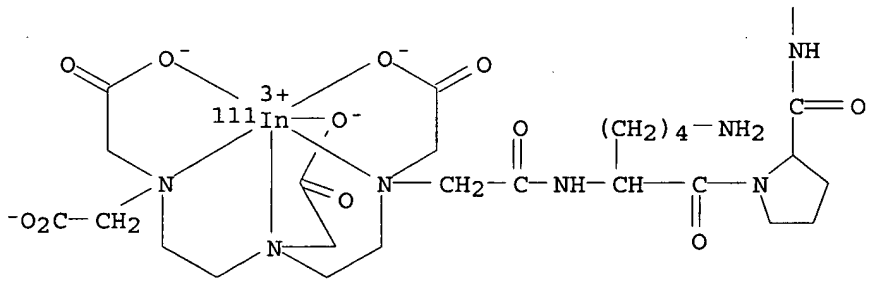

● 2 H^+

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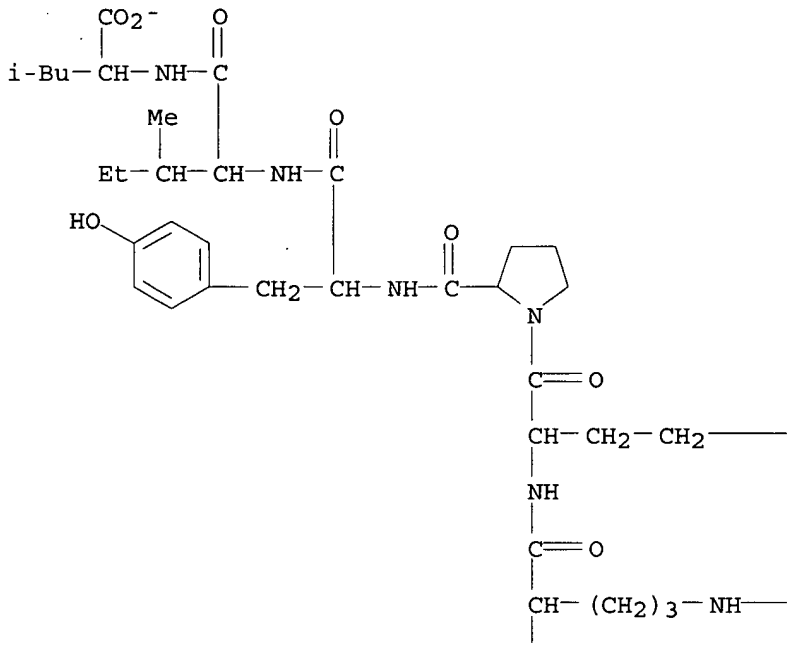
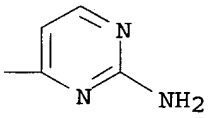
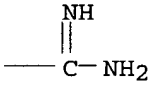
PAGE 1-A

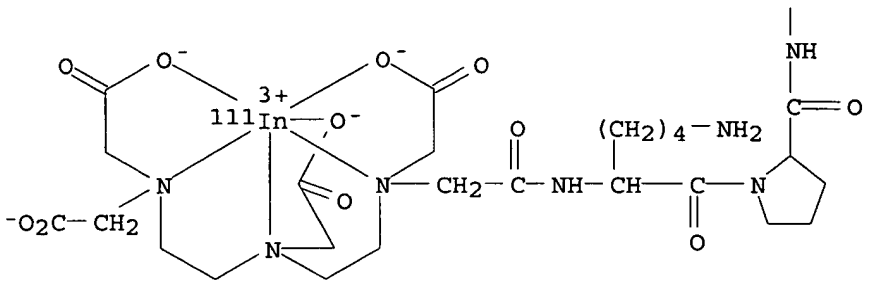


PAGE 1-B





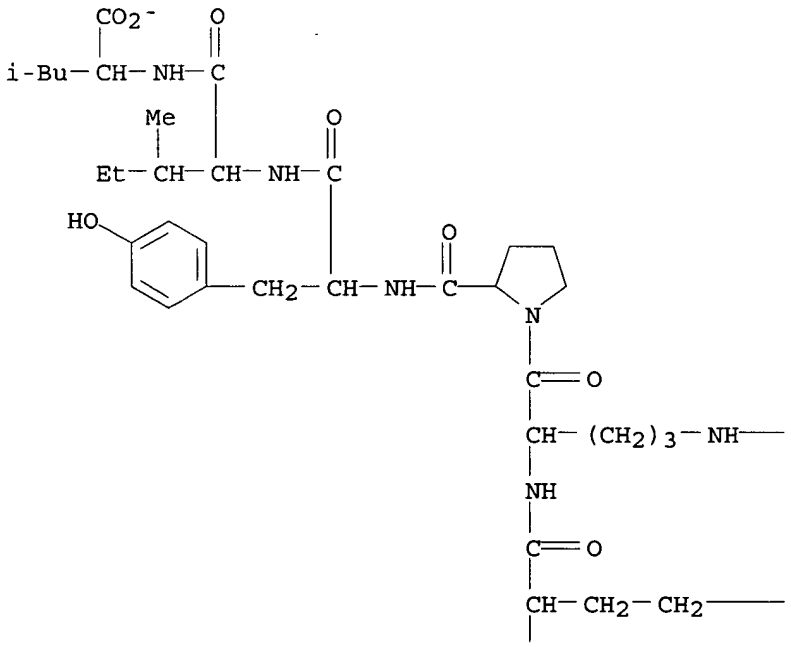
PAGE 2-A



●2 H+

RN 328526-81-4 CAPLUS
CN Indate(2-)-111In, [N-[(carboxy-κO)methyl]-N-[2-[[(carboxy-κO)methyl][2-[[(carboxy-κO)methyl](carboxymethyl)amino-κN]ethyl]amino-κN]ethyl]glycyl-κN-D-lysyl-L-prolyl-(αS)-α,2-diamino-4-pyrimidinebutanoyl-L-arginyl-L-prolyl-L-tyrosyl-L-isoleucyl-L-leucinato(5-)]-, dihydrogen (9CI) (CA INDEX NAME)

PAGE 1-A



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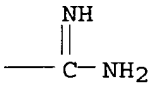

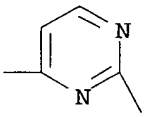

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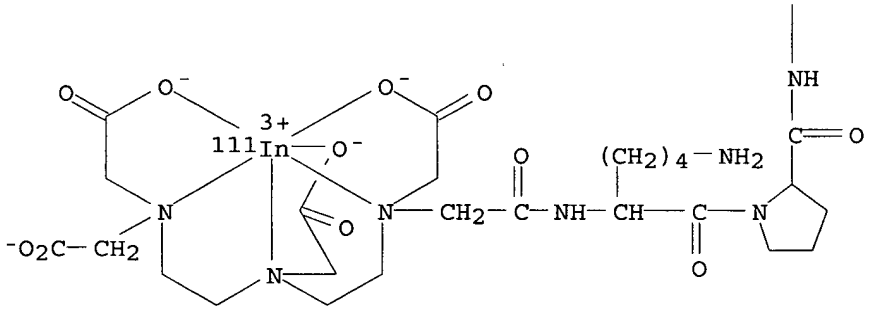

● 2 H^+

PAGE 2-B

RN 328526-82-5 CAPLUS
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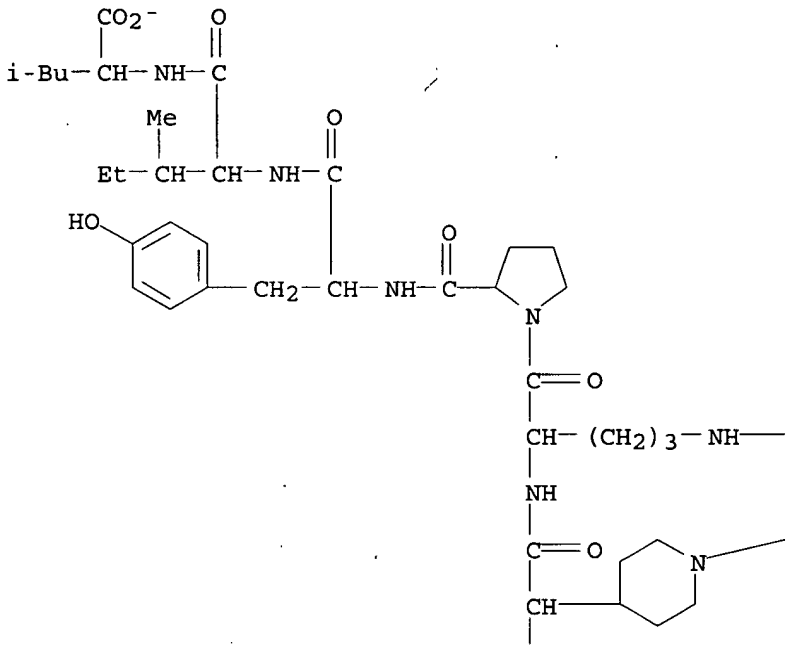
Searched by Barb O'Bryen, STIC 2-2518

2-[1-(aminoiminomethyl)-4-piperidinyl]glycyl-L-arginyl-L-prolyl-L-tyrosyl-L-isoleucyl-L-leucinato(5-)]-, dihydrogen (9CI) (CA INDEX NAME)

PAGE 1-A



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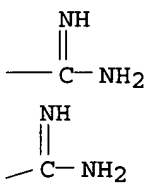

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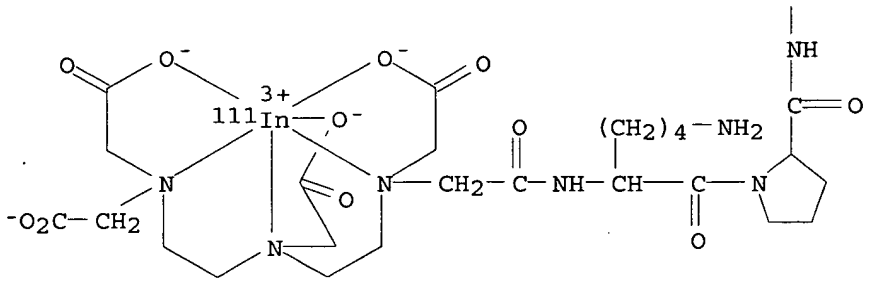

●2 H^+

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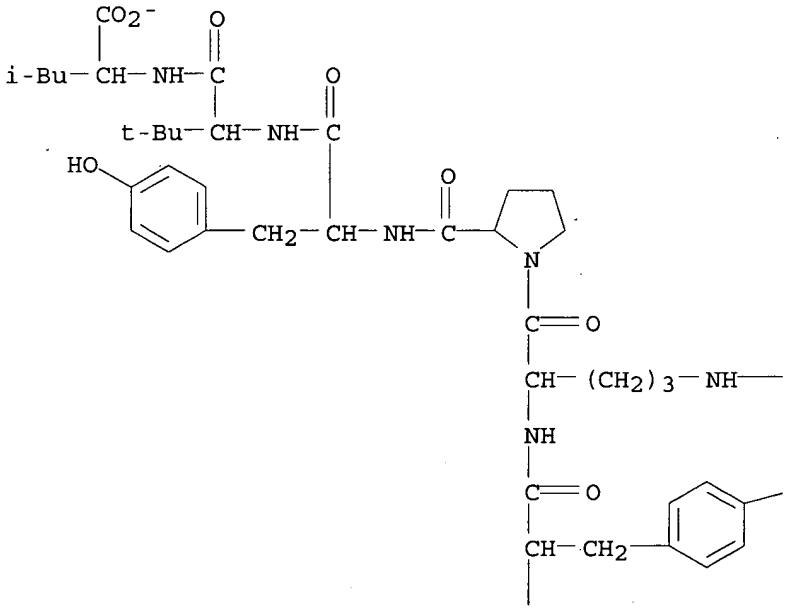
PAGE 1-A



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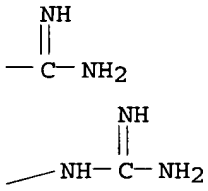

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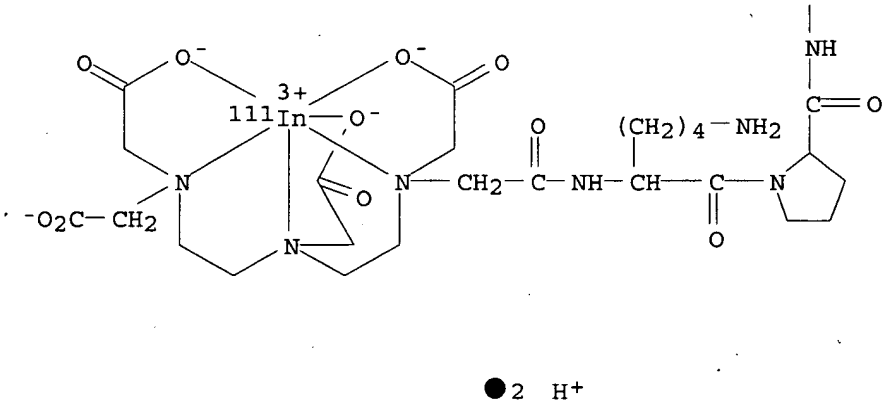

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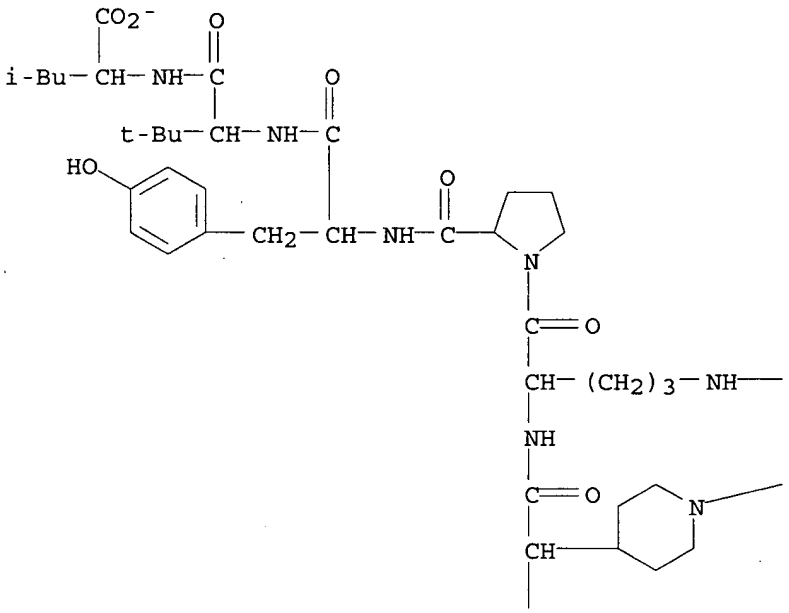
PAGE 1-A



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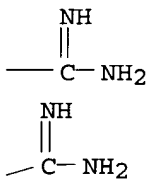
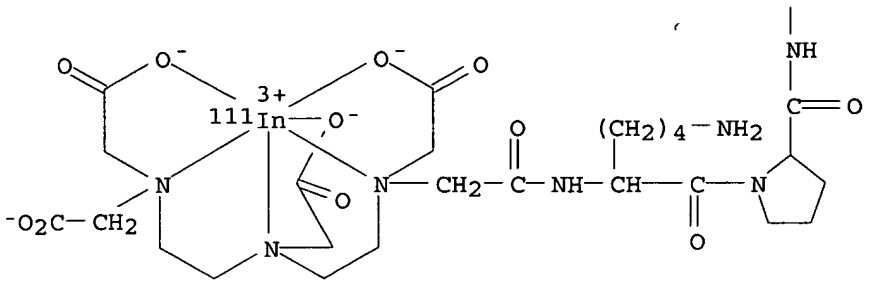


PAGE 2-A

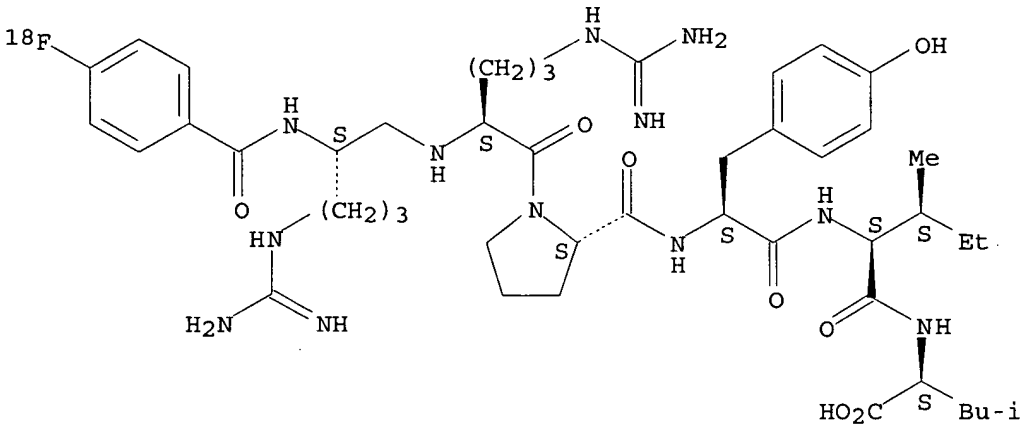


●2 H+

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L45 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:64319 CAPLUS
DOCUMENT NUMBER: 132:322121
TITLE: Reaction of neurotensin (8-13) and its partially reduced congener with unlabeled and 18F-labeled N-succinimidyl 4-fluorobenzoate (SFB)
AUTHOR(S): Scheunemann, M.; Mading, P.; Bergmann, R.; Steinbach, J.; Johannsen, B.; Tourwe, D.
CORPORATE SOURCE: Vrije Universiteit Brussel, Belg.
SOURCE: Wissenschaftlich-Technische Berichte - Forschungszentrum Rossendorf (1999), FZR-270, 26-28
CODEN: WBFRFQ; ISSN: 1437-322X
DOCUMENT TYPE: Report
LANGUAGE: German
ED Entered STN: 27 Jan 2000
AB Labeling expts. with neurotensin (NT) (8-13) and partially reduced congener [Arg8Ψ(CH2NH)Arg9]NT(8-13) as well as arginine and Arg-Tyr were performed using N-succinimidyl fluorobenzoate (SFB)and [18F]SFB. The labeling expts. revealed that [18F]SFB reacts with N-terminal Arg-peptides with reasonably good chemoselectivity in aqueous buffered solns., preferably at pH 8.3.
IT **266352-47-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(reaction of neurotensin with unlabeled and 18F-labeled succinimidyl fluorobenzoate)
RN 266352-47-0 CAPLUS
CN L-Leucine, N2-[(2S)-5-[(aminoiminomethyl)amino]-2-[[4-(fluoro-18F)benzoyl]amino]pentyl]-L-arginyl-L-prolyl-L-tyrosyl-L-isoleucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L45 ANSWER 11 OF 11 PROUSDDR COPYRIGHT 2005 PROUS SCIENCE on STN
ACCESSION NUMBER: 2003:6476 PROUSDDR
DOCUMENT NUMBER: 343678
CHEMICAL NAME: (N-(2-(N-(2-(N,N-Bis(carboxymethyl)amino)ethyl)-N-(carboxymethyl)amino)ethyl)-N-(carboxymethyl)glycyl-2-(4-piperidinyl)-L-glycyl-L-prolyl-2-(1-amidinopiperidin-4-yl)-L-glycyl-L-arginyl-L-prolyl-L-tyrosyl-3-methyl-L-valyl-L-leucinato(3-))indium-111In
CAS REGISTRY NUMBER: **314295-66-4** (uncomplexed)
MOLECULAR FORMULA: C66 H103 N18 O19 . In
HIGHEST DEV. PHASE: PRECLINICAL
ORIGINATOR: Mallinckrodt
CLASSIFICATION CODE: Diagnostic for Cancer; Drug Delivery Systems
ENTRY DATE: Entered STN: 9 May 2004
Last Updated on STN: 9 May 2004

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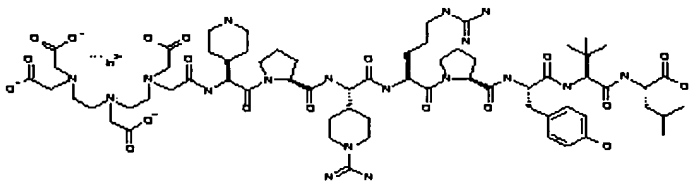

PROUS REFERENCES:
RefID: 745062 (Text Available)
Drug Data Report, Vol. 25, No. 8, pp 766, 2003

REFERENCE TEXT: RefID: 745062
ACTION -111In-Labeled DTPA-neurotensin peptide analogue conjugate for the delivery of cytotoxic and imaging agents to tumors. It showed high binding affinity for the neurotensin receptor in human

adenocarcinoma HT-29 cells (IC50 = 0.3 nM) and high metabolic stability in human serum and rat urine. Studies in SCID mice bearing neurotensin receptor-positive HT-29 xenografts demonstrated selective uptake of compound by tumor tissue following i.v. administration via a neurotensin receptor-specific mechanism.

PATENT REFERENCES:

TITLE:	Labeled neurotensin derivs.
INVENTOR(S):	Srinivasan, A.; Erion, J.L.; Schmidt, M.A.
PATENT ASSIGNEE(S):	Mallinckrodt
PATENT INFORMATION:	EP 1194444 20020410
	WO 2000078796 20001228
PRIORITY INFORMATION:	US 1999-140913 19990624
	US 2000-213068 20000621

REFERENCES:

(1) RefID: 744694, Periodic Publication
"Novel bioactive and stable neurotensin peptide analogues capable of delivering radiopharmaceuticals and molecular beacons to tumors" Achilefu, S.; Srinivasan, A.; Schmidt, M.A.; Jimenez, H.N.; Bugaj, J.E.; Erion, J.L., J Med Chem, Vol. 46, No. 15, pp 3403, 2003

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